



## Full wwPDB EM Validation Report ⓘ

Jun 17, 2025 – 12:01 AM JST

PDB ID : 7DR6 / pdb\_00007dr6  
EMDB ID : EMD-30824  
Title : PA28alpha-beta in complex with immunoproteasome  
Authors : Cong, Y.; Xu, C.  
Deposited on : 2020-12-26  
Resolution : 4.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

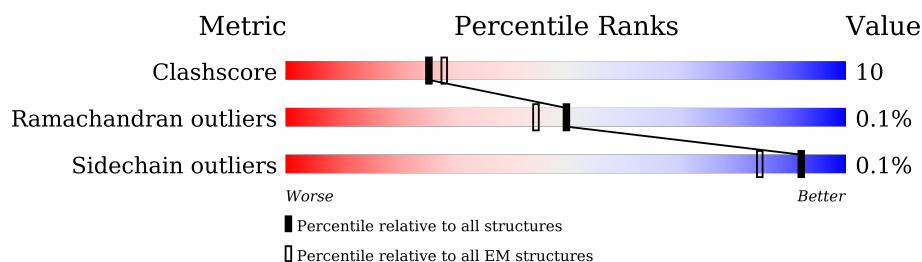
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	246	<div> <div>21%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
1	e	246	<div> <div>34%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>
2	M	234	<div> <div>22%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
2	f	234	<div> <div>26%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
3	N	261	<div> <div>26%</div> <div>72%</div> <div>23%</div> <div>6%</div> </div>
3	g	261	<div> <div>30%</div> <div>73%</div> <div>21%</div> <div>6%</div> </div>
4	O	248	<div> <div>31%</div> <div>69%</div> <div>24%</div> <div>6%</div> </div>
4	a	248	<div> <div>30%</div> <div>68%</div> <div>25%</div> <div>6%</div> </div>



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Mol	Chain	Length	Quality of chain
5	P	241	
5	b	241	
6	Q	263	
6	c	263	
7	R	255	
7	d	255	
8	A	239	
8	D	239	
8	F	239	
9	B	249	
9	C	249	
9	E	249	
9	G	249	
10	H	205	
10	S	205	
11	I	201	
11	T	201	
12	J	241	
12	U	241	
13	K	264	
13	V	264	
14	W	219	
14	Z	219	
15	1	273	
15	X	273	

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Mol	Chain	Length	Quality of chain
16	2	276	
16	Y	276	

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 59957 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	236	Total	C	N	O	S	0	0
			1850	1178	306	353	13		
1	e	238	Total	C	N	O	S	0	0
			1856	1181	308	354	13		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	226	Total	C	N	O	S	0	0
			1763	1127	298	332	6		
2	f	230	Total	C	N	O	S	0	0
			1793	1147	302	338	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	246	Total	C	N	O	S	0	0
			1936	1225	331	369	11		
3	g	246	Total	C	N	O	S	0	0
			1936	1225	331	369	11		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	232	Total	C	N	O	S	0	0
			1824	1149	322	348	5		
4	a	232	Total	C	N	O	S	0	0
			1824	1149	322	348	5		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	234	Total	C	N	O	S	0	0
			1790	1125	295	359	11		
5	b	234	Total	C	N	O	S	0	0
			1790	1125	295	359	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	235	Total	C	N	O	S	0	0
			1846	1156	330	349	11		
6	c	235	Total	C	N	O	S	0	0
			1846	1156	330	349	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	240	Total	C	N	O	S	0	0
			1879	1191	321	356	11		
7	d	240	Total	C	N	O	S	0	0
			1879	1191	321	356	11		

- Molecule 8 is a protein called Proteasome activator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	209	Total	C	N	O	S	0	0
			1684	1084	286	310	4		
8	D	207	Total	C	N	O	S	0	0
			1678	1080	283	311	4		
8	F	210	Total	C	N	O	S	0	0
			1695	1091	287	313	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	PRO	HIS	variant	UNP Q9UL46
D	89	PRO	HIS	variant	UNP Q9UL46
F	89	PRO	HIS	variant	UNP Q9UL46

- Molecule 9 is a protein called Proteasome activator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	213	Total	C	N	O	S	0	0
			1720	1102	292	320	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	206	Total	C	N	O	S	0	0
			1663	1063	284	310	6		
9	E	208	Total	C	N	O	S	0	0
			1685	1078	287	314	6		
9	G	205	Total	C	N	O	S	0	0
			1654	1057	283	306	8		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	204	Total	C	N	O	S	0	0
			1594	1015	265	295	19		
10	S	204	Total	C	N	O	S	0	0
			1594	1015	265	295	19		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	198	Total	C	N	O	S	0	0
			1593	1023	270	292	8		
11	T	197	Total	C	N	O	S	0	0
			1584	1017	268	291	8		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	213	Total	C	N	O	S	0	0
			1645	1042	282	311	10		
12	U	213	Total	C	N	O	S	0	0
			1645	1042	282	311	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	216	Total	C	N	O	S	0	0
			1685	1065	289	319	12		
13	V	216	Total	C	N	O	S	0	0
			1682	1063	289	318	12		

- Molecule 14 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	199	Total	C	N	O	S	0	0
			1500	942	257	291	10		
14	Z	199	Total	C	N	O	S	0	0
			1500	942	257	291	10		

- Molecule 15 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	219	Total	C	N	O	S	0	0
			1611	1010	281	309	11		
15	1	219	Total	C	N	O	S	0	0
			1611	1010	281	309	11		

- Molecule 16 is a protein called Proteasome subunit beta type-8.

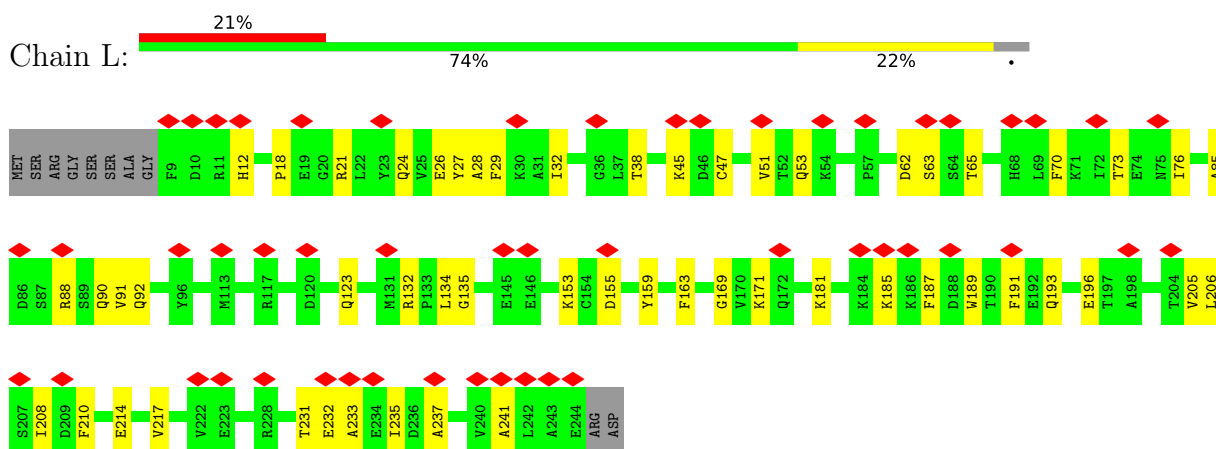
Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	201	Total	C	N	O	S	0	0
			1561	975	273	297	16		
16	2	201	Total	C	N	O	S	0	0
			1561	975	273	297	16		



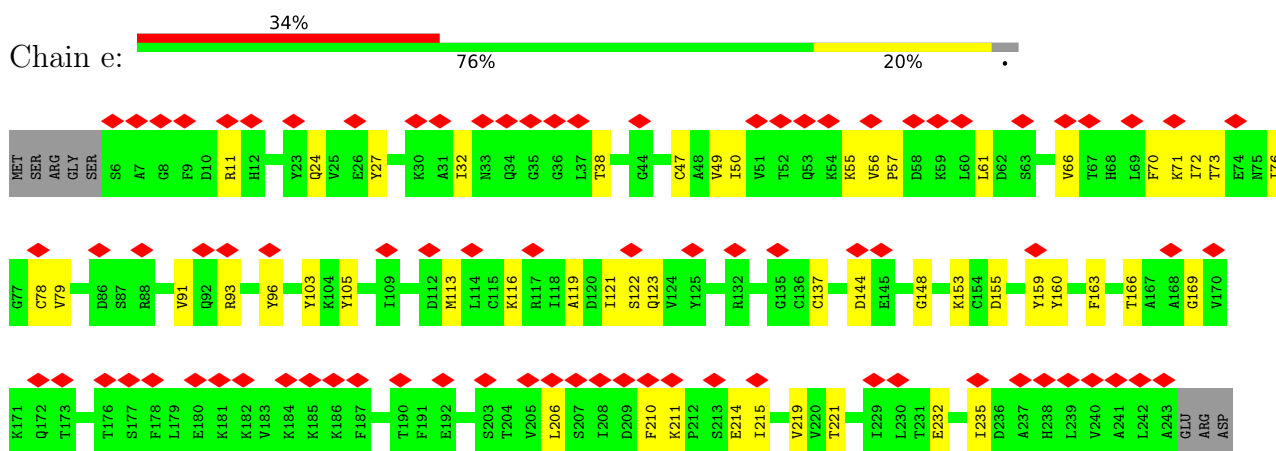
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

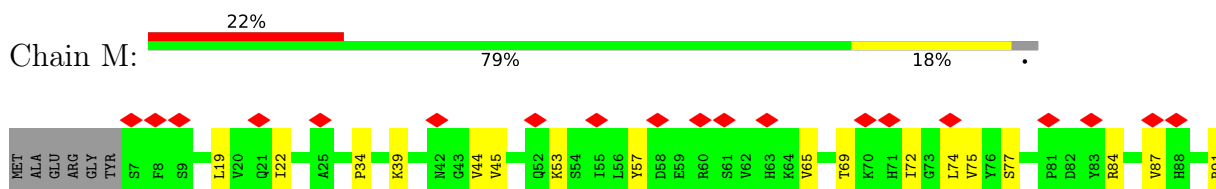
- Molecule 1: Proteasome subunit alpha type-6

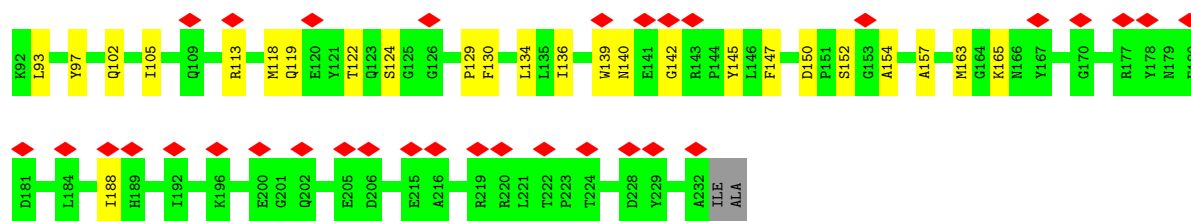


- Molecule 1: Proteasome subunit alpha type-6



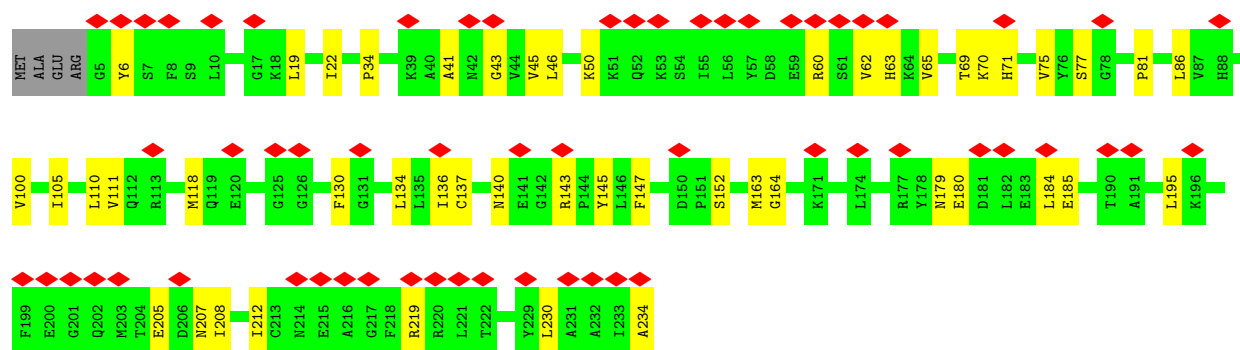
- Molecule 2: Proteasome subunit alpha type-2





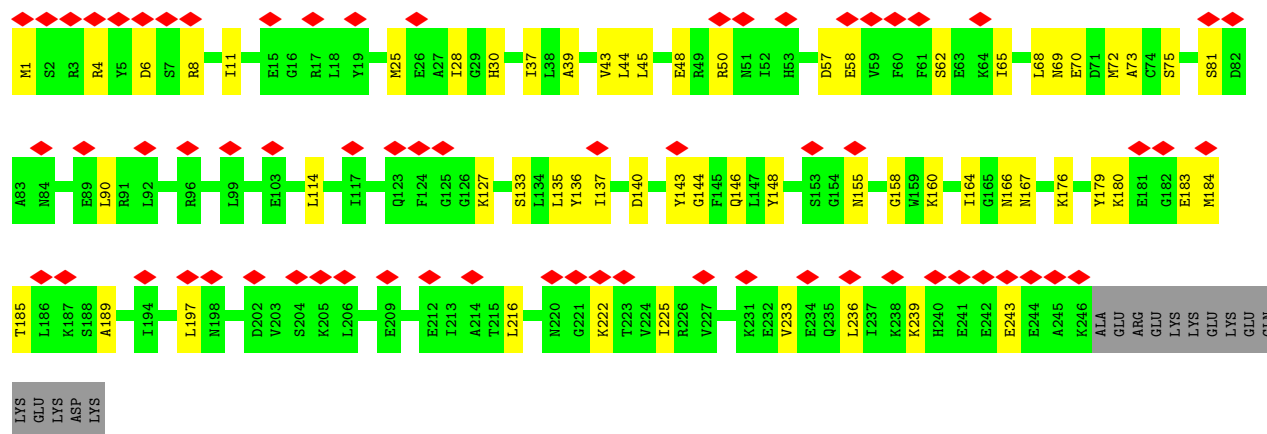
• Molecule 2: Proteasome subunit alpha type-2

Chain f: 26% 78% 21% .



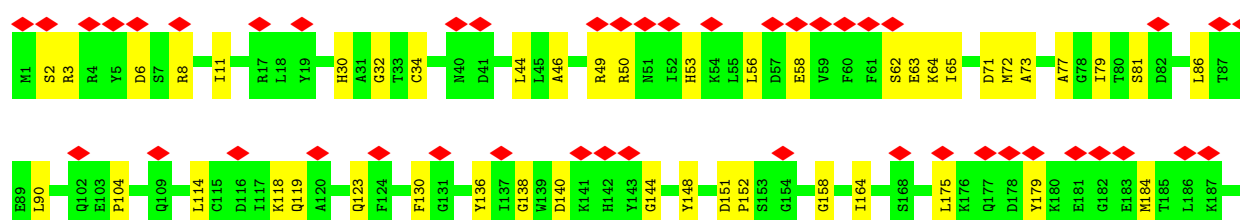
• Molecule 3: Proteasome subunit alpha type-4

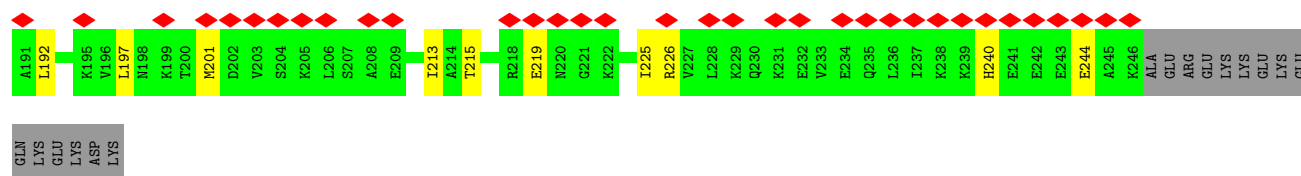
Chain N: 26% 72% 23% 6%



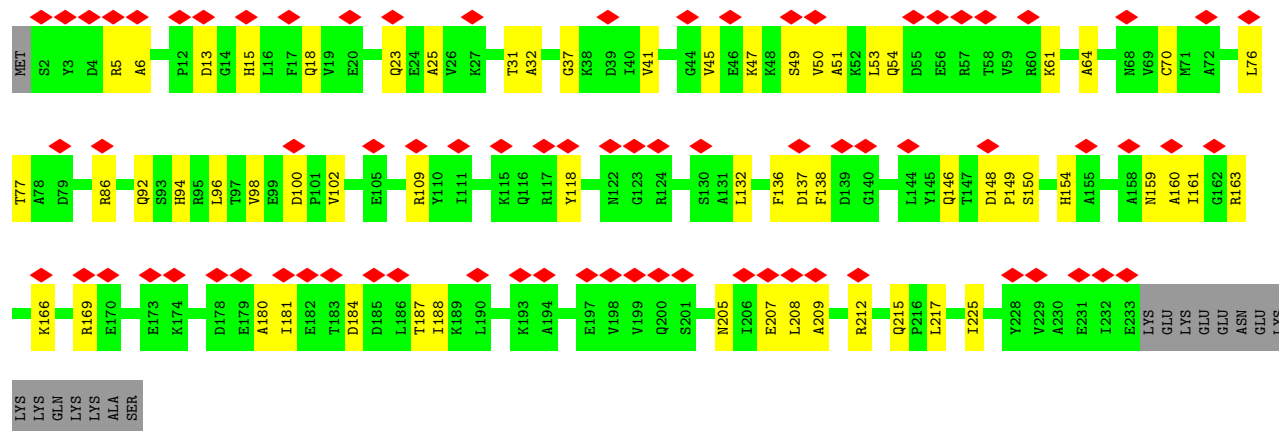
• Molecule 3: Proteasome subunit alpha type-4

Chain g: 30% 73% 21% 6%

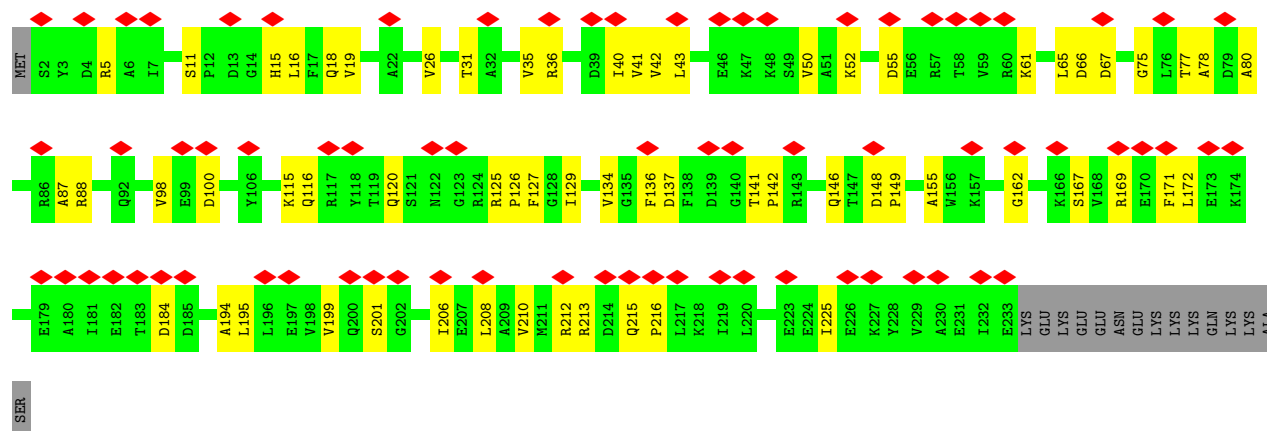




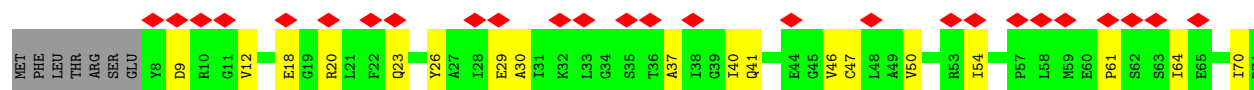
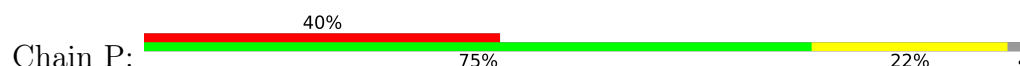
• Molecule 4: Proteasome subunit alpha type-7

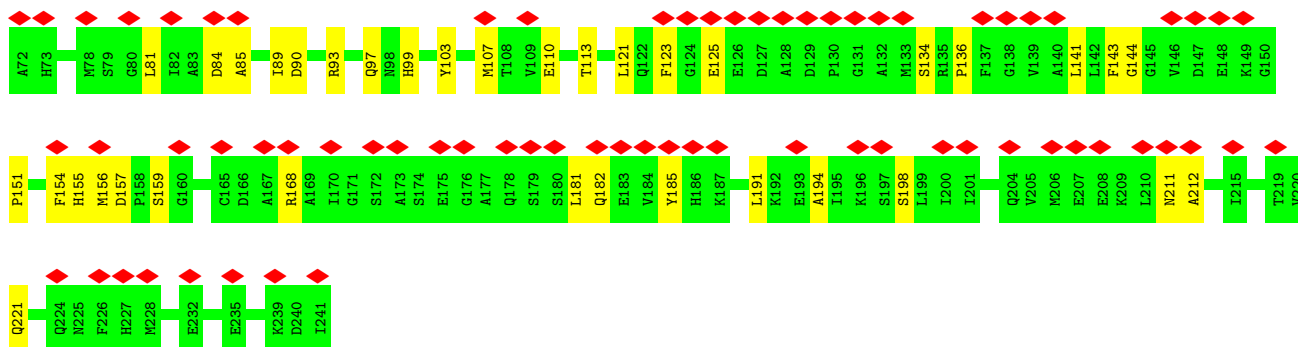


• Molecule 4: Proteasome subunit alpha type-7



• Molecule 5: Proteasome subunit alpha type-5

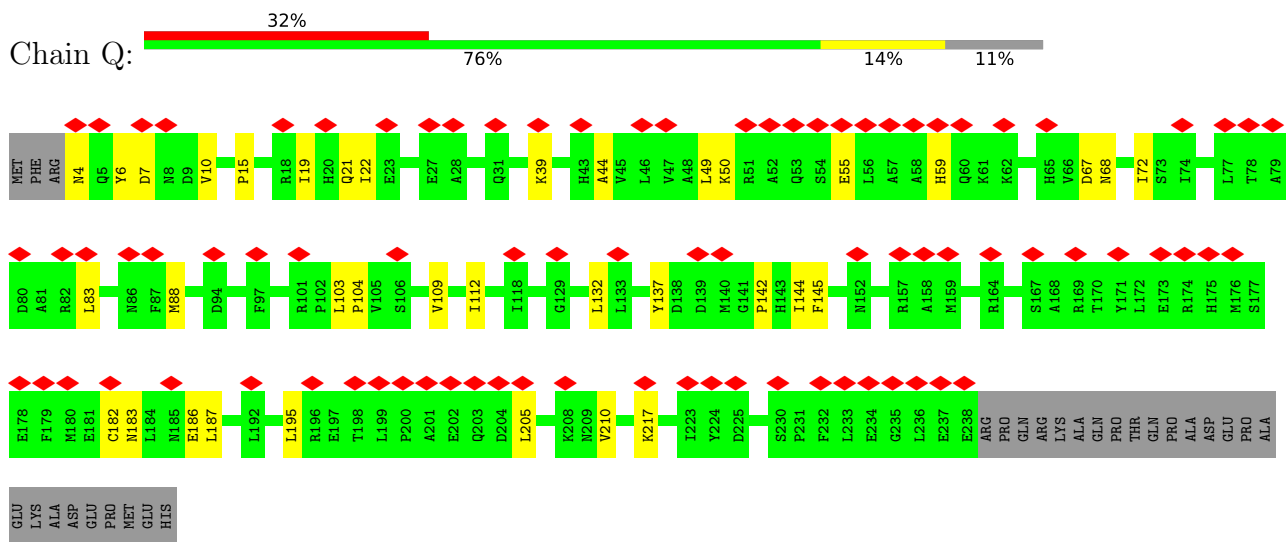




• Molecule 5: Proteasome subunit alpha type-5

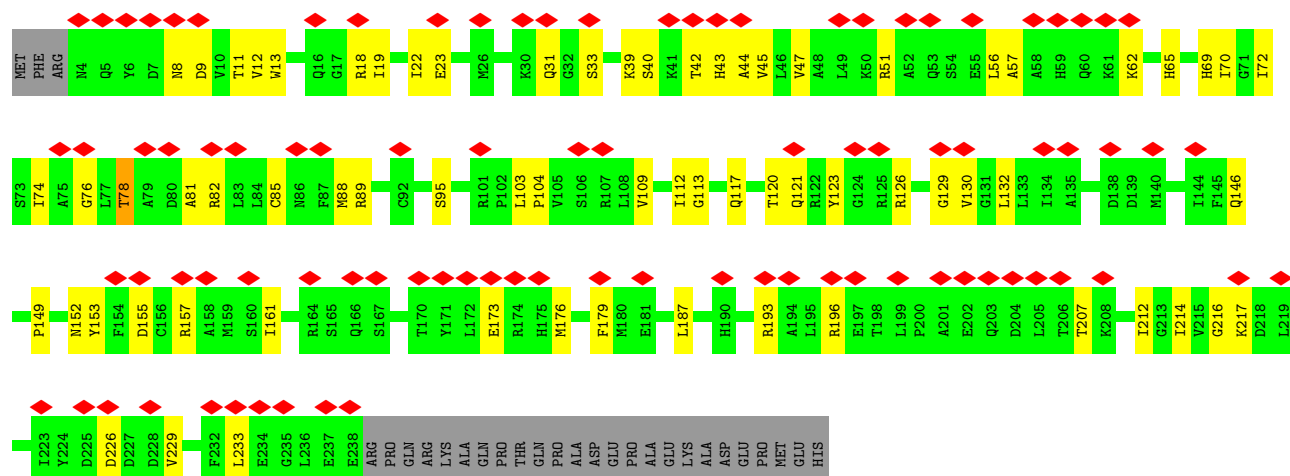


• Molecule 6: Proteasome subunit alpha type-1

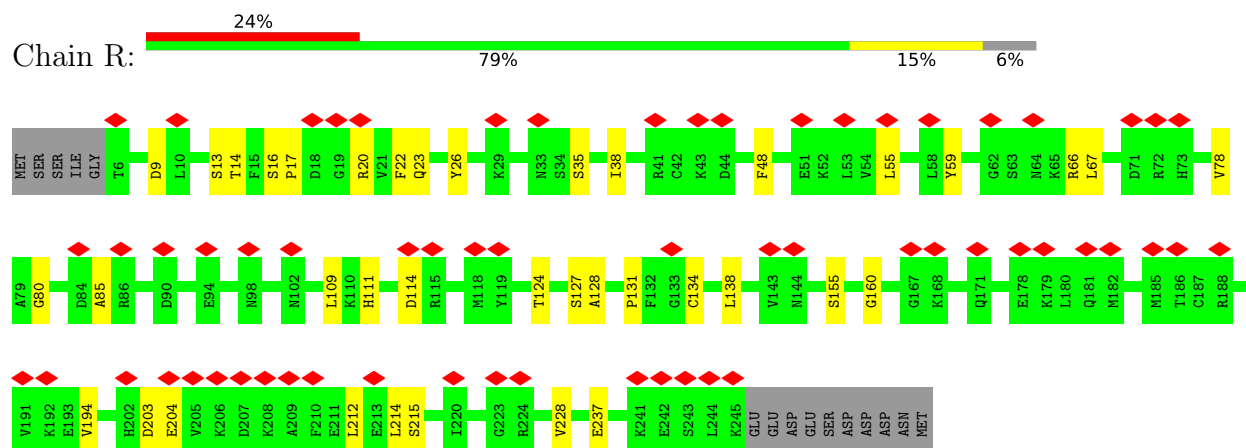


• Molecule 6: Proteasome subunit alpha type-1



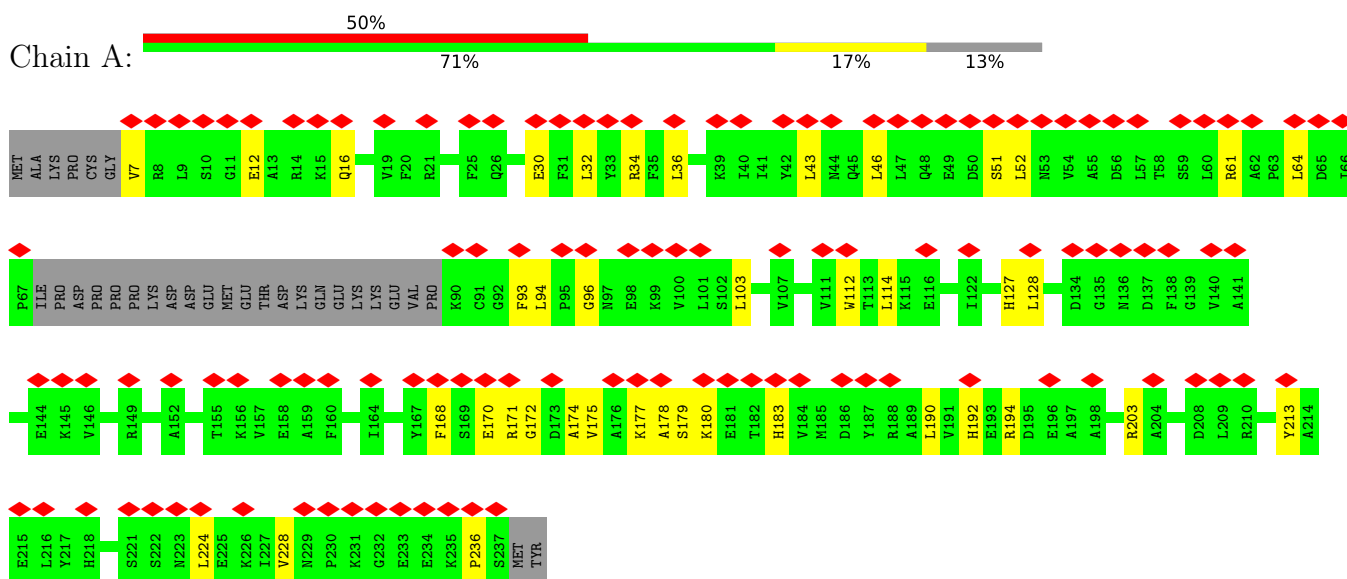


- Molecule 7: Proteasome subunit alpha type-3

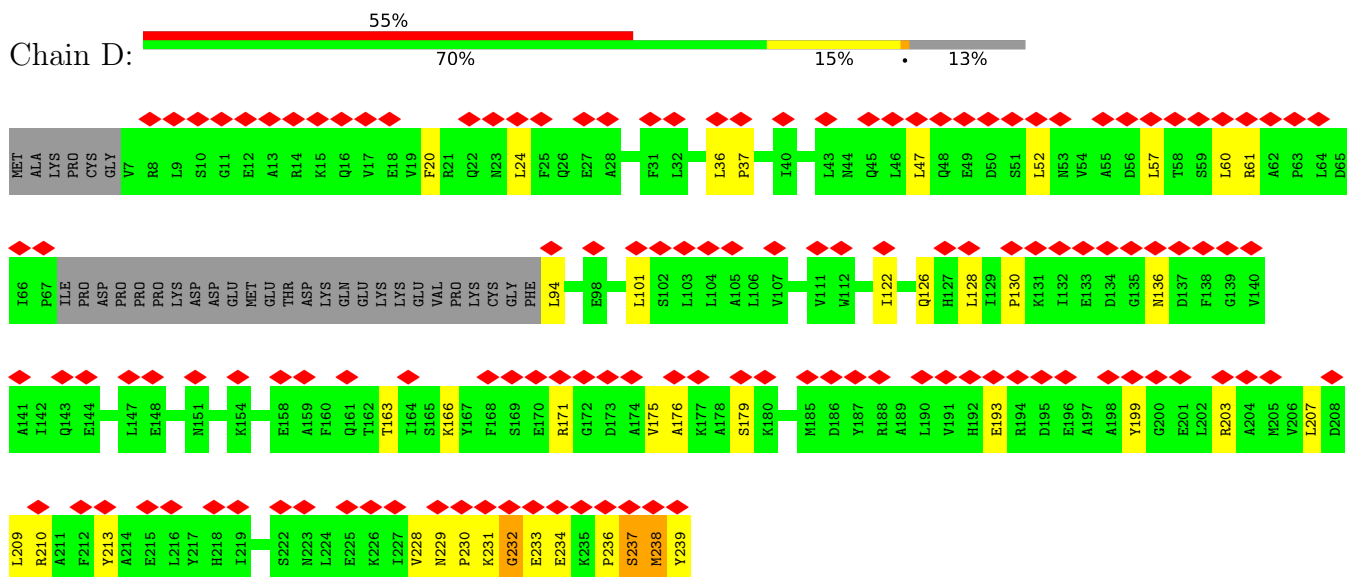


- Molecule 8: Proteasome activator complex subunit 2

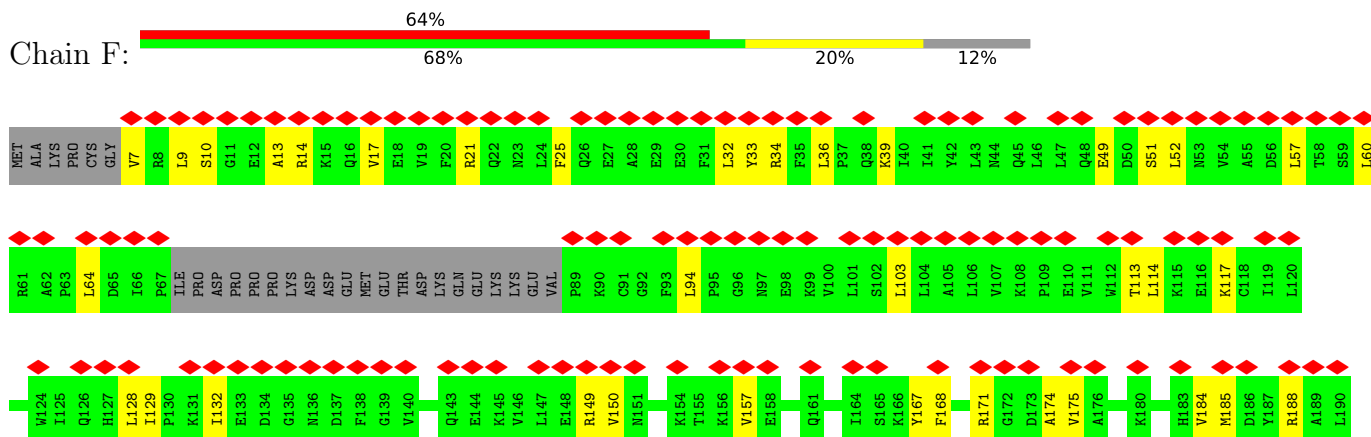


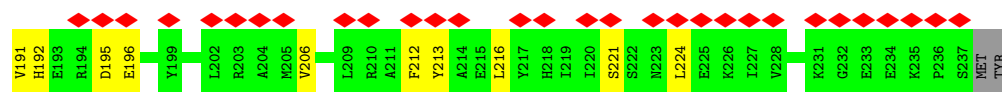


• Molecule 8: Proteasome activator complex subunit 2

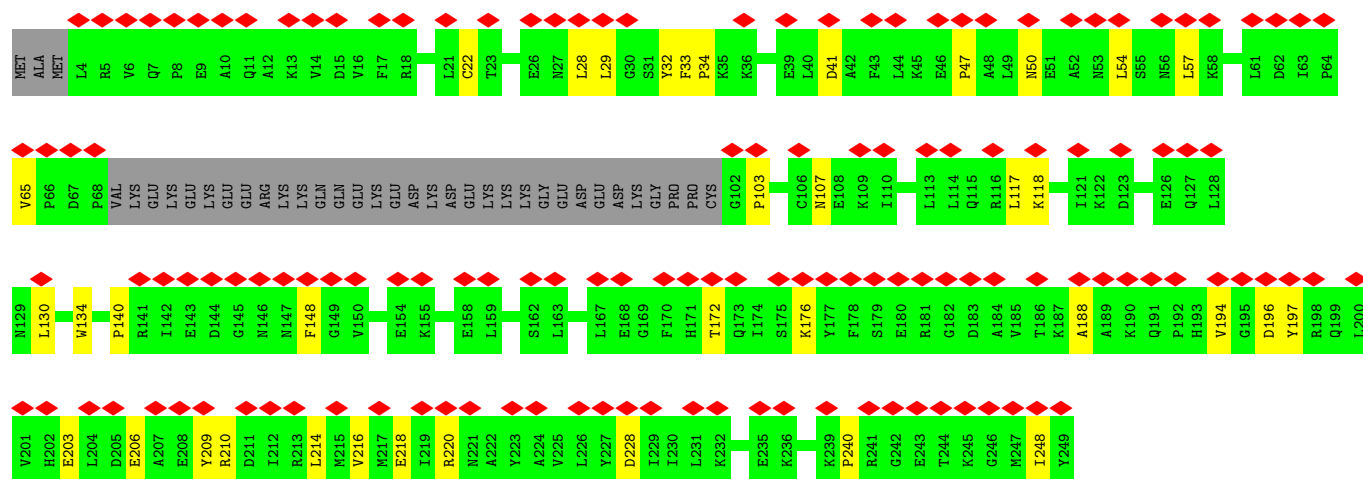
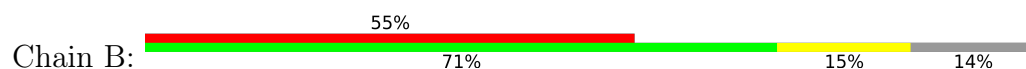


• Molecule 8: Proteasome activator complex subunit 2

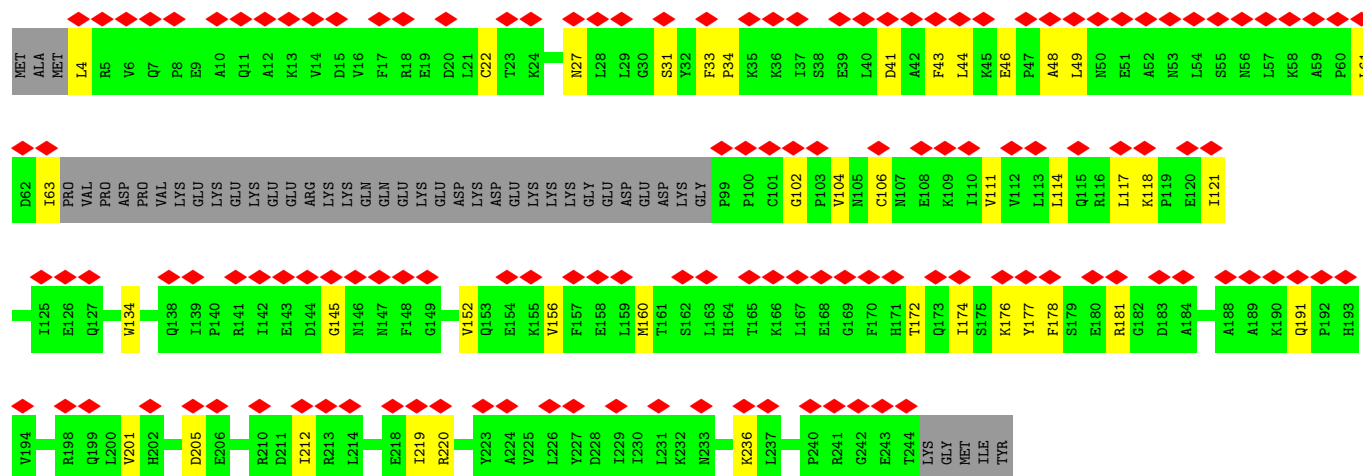




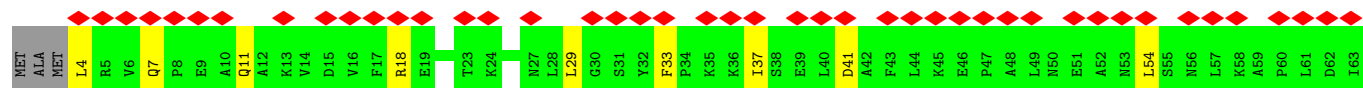
• Molecule 9: Proteasome activator complex subunit 1

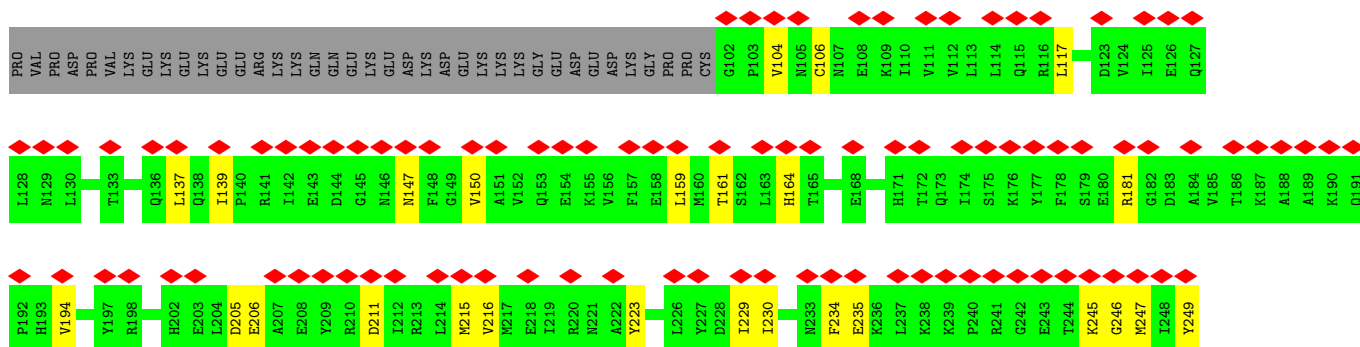


• Molecule 9: Proteasome activator complex subunit 1

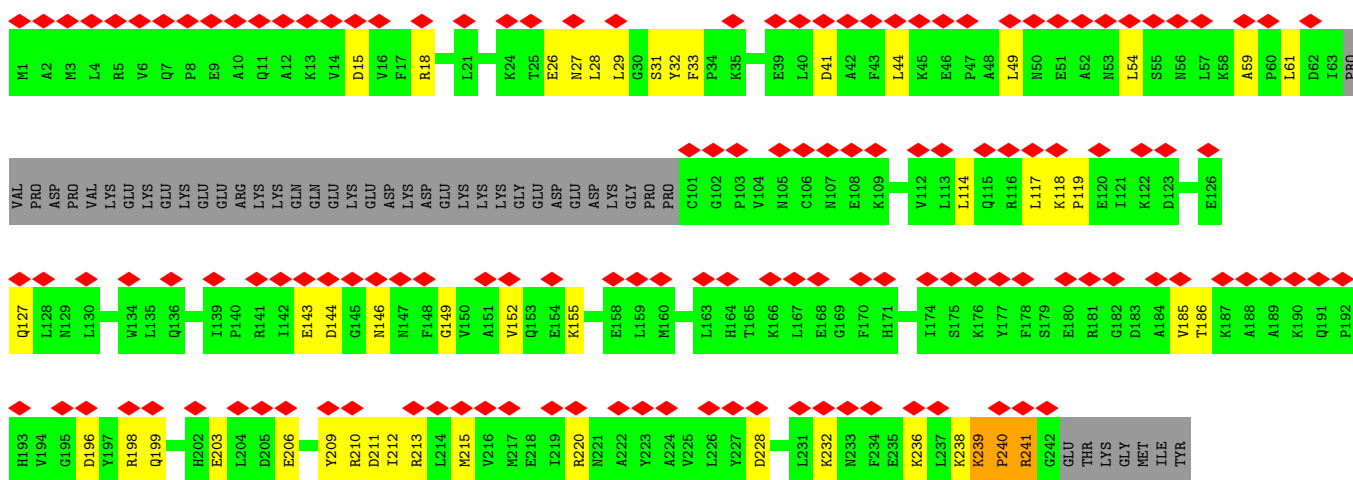


• Molecule 9: Proteasome activator complex subunit 1

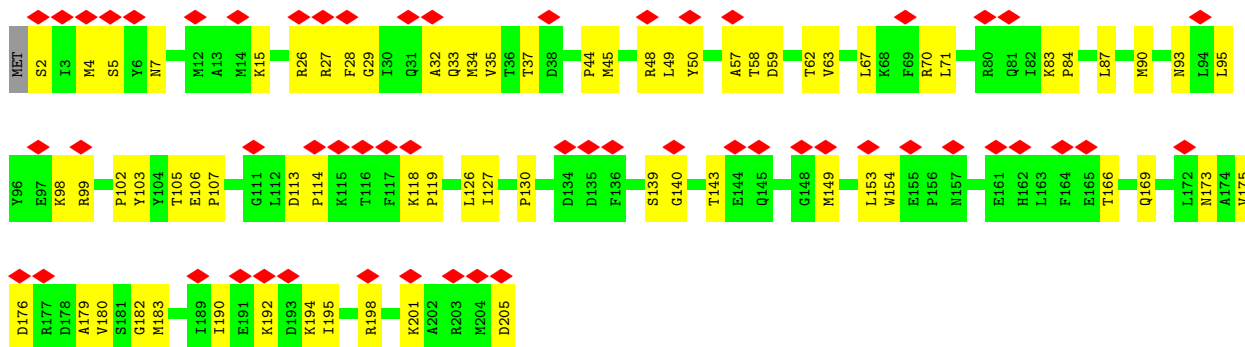




• Molecule 9: Proteasome activator complex subunit 1



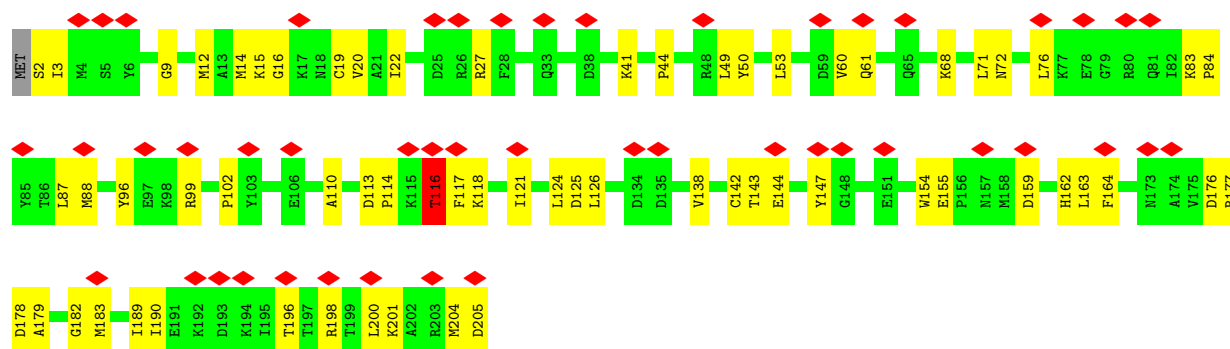
• Molecule 10: Proteasome subunit beta type-3



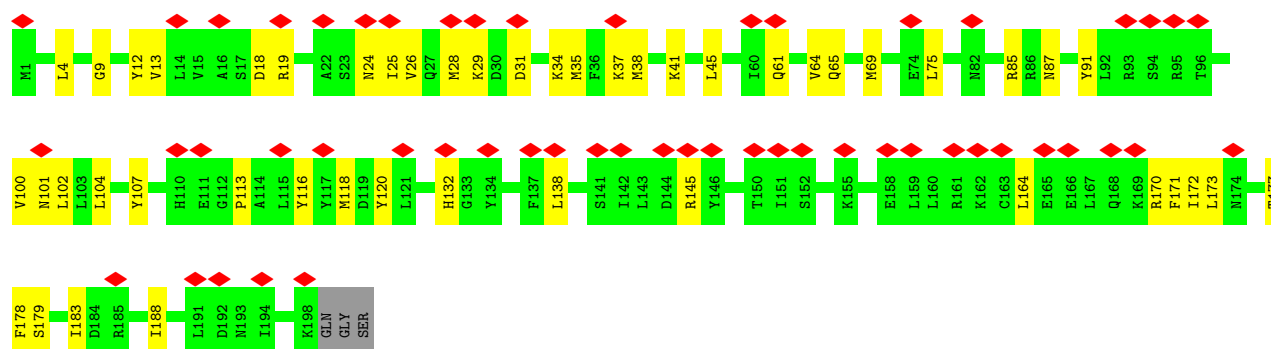
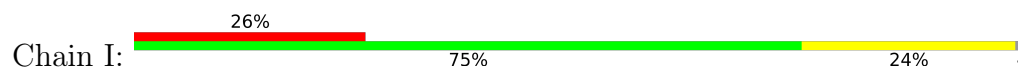
• Molecule 10: Proteasome subunit beta type-3



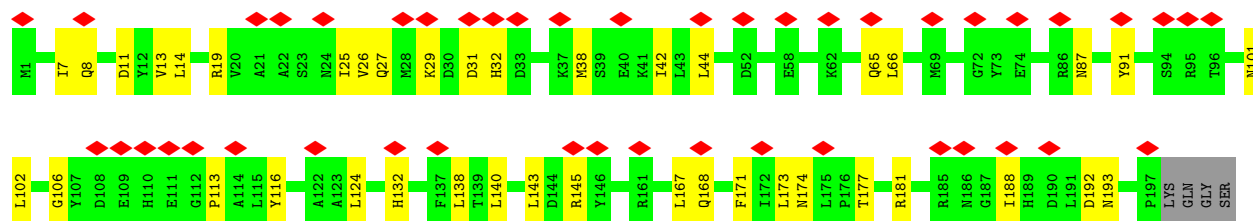
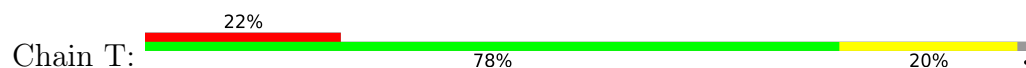




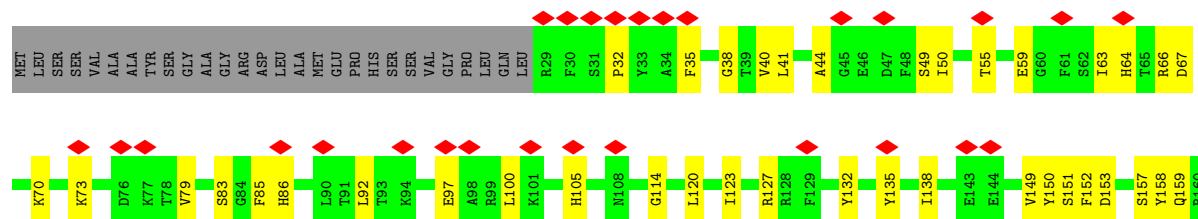
• Molecule 11: Proteasome subunit beta type-2

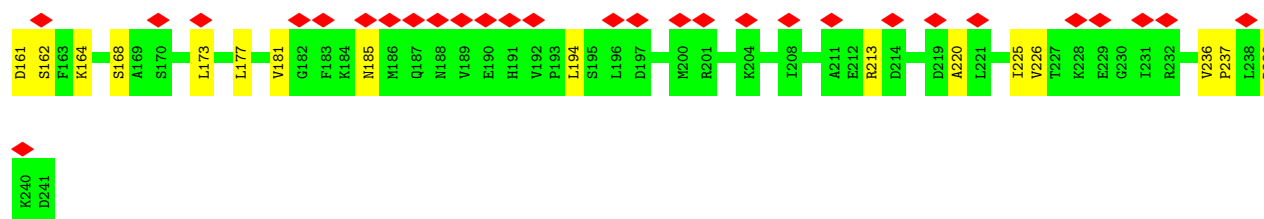


• Molecule 11: Proteasome subunit beta type-2

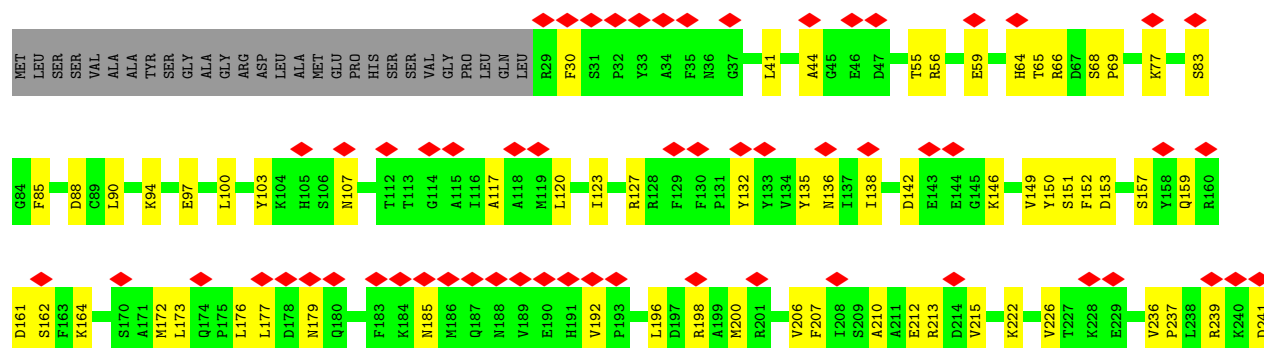


• Molecule 12: Proteasome subunit beta type-1

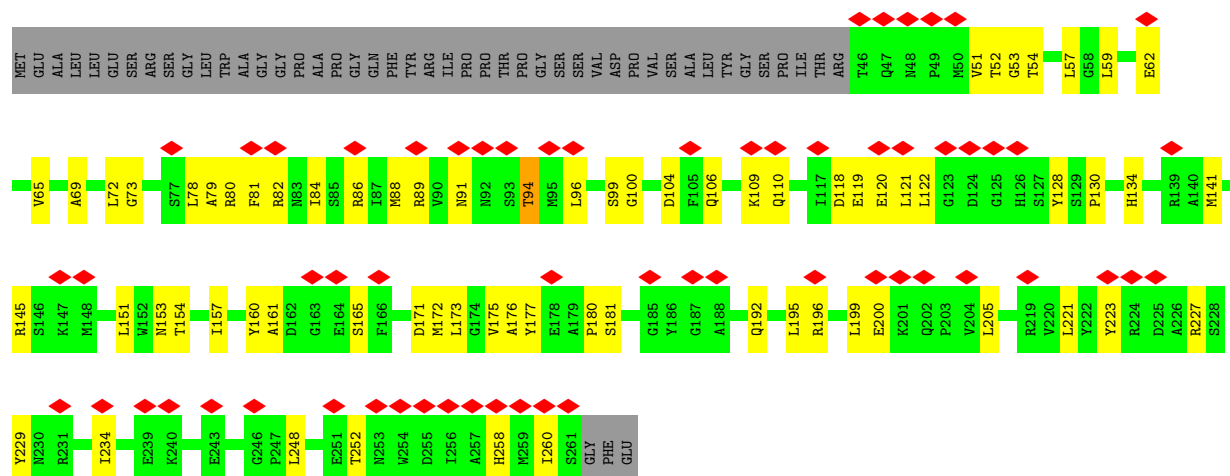




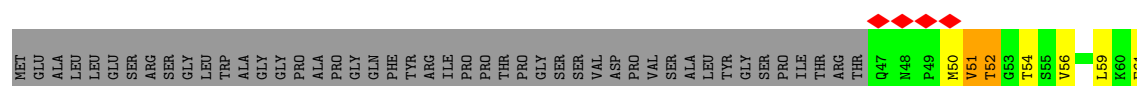
• Molecule 12: Proteasome subunit beta type-1

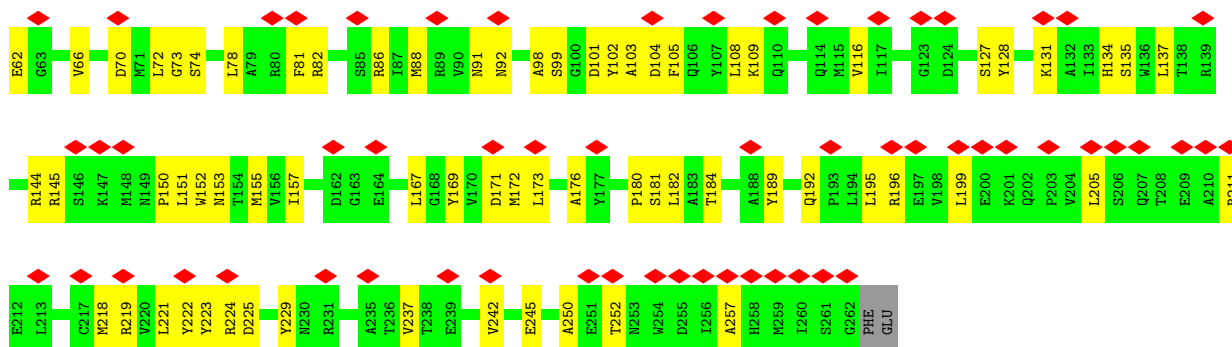


• Molecule 13: Proteasome subunit beta type-4

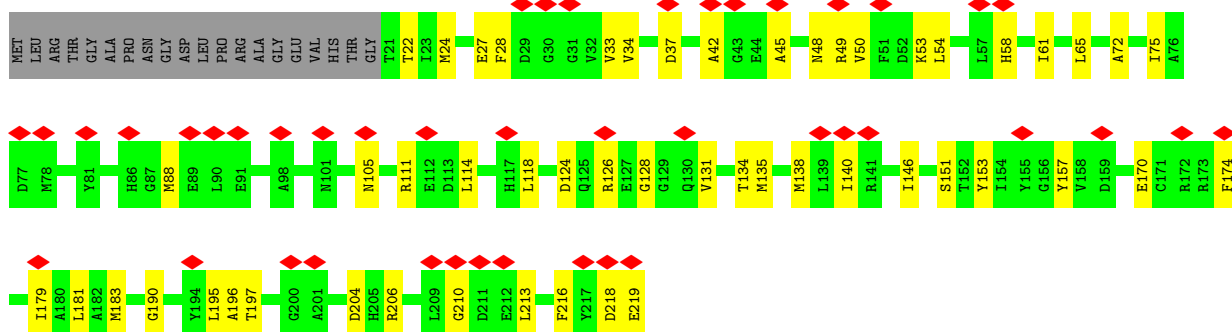


• Molecule 13: Proteasome subunit beta type-4

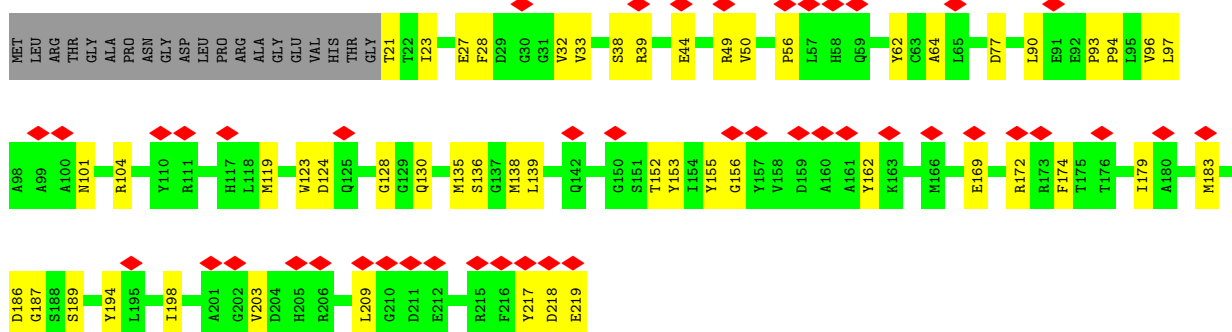




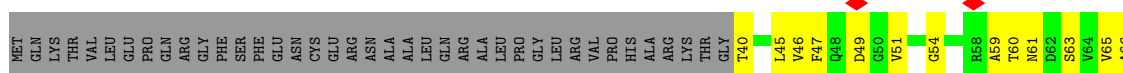
• Molecule 14: Proteasome subunit beta type-9

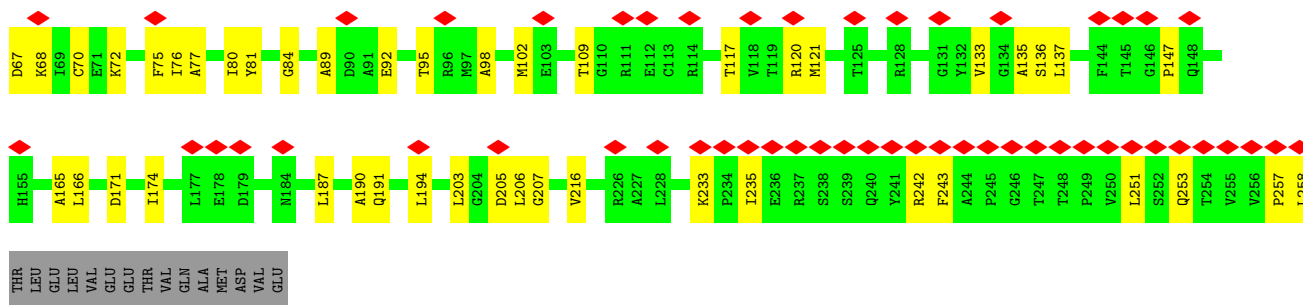


• Molecule 14: Proteasome subunit beta type-9

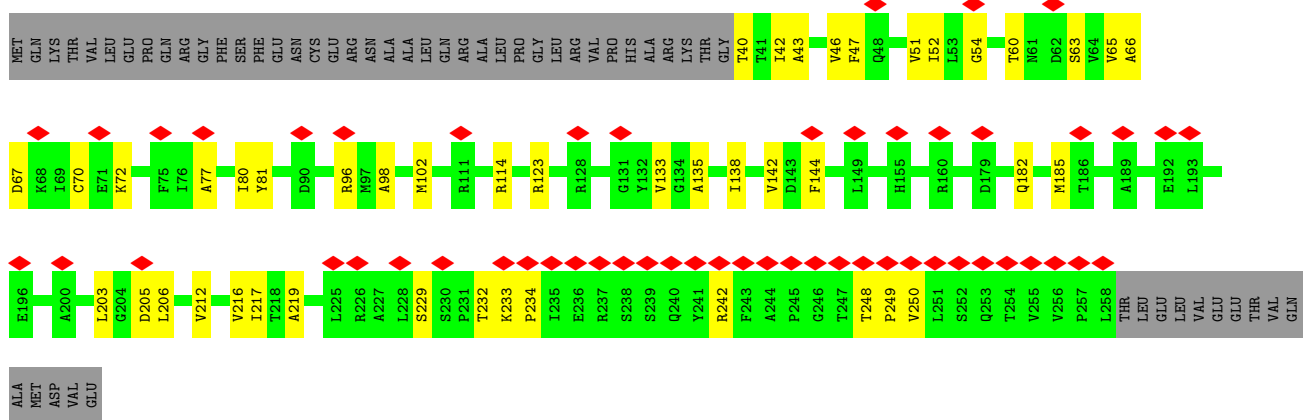


• Molecule 15: Proteasome subunit beta type-10

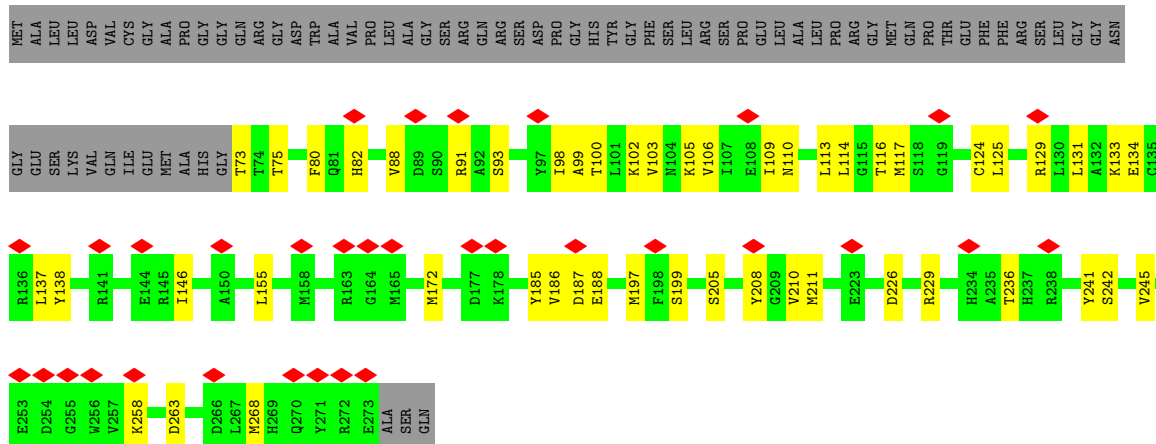




• Molecule 15: Proteasome subunit beta type-10

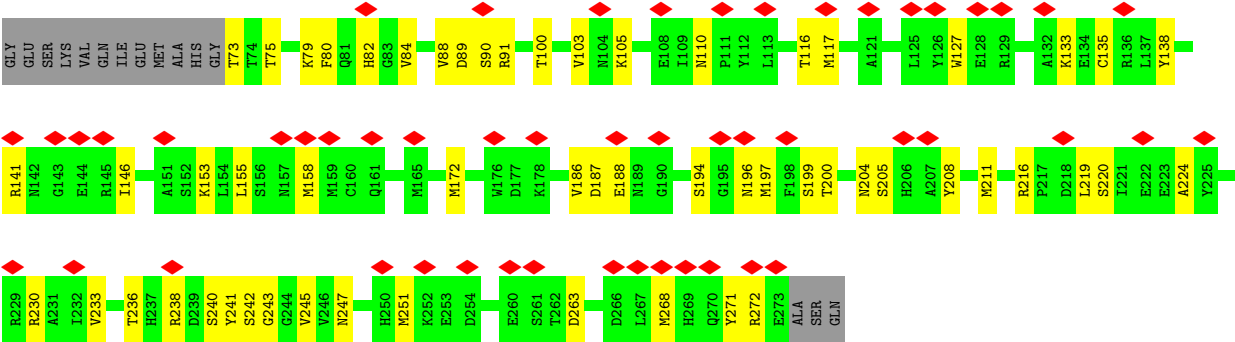


• Molecule 16: Proteasome subunit beta type-8



• Molecule 16: Proteasome subunit beta type-8





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45030	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.322	Depositor
Minimum map value	-1.426	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.619	Depositor
Map size (Å)	337.408, 337.408, 337.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	L	0.11	0/1884	0.36	0/2548
1	e	0.11	0/1890	0.35	0/2556
2	M	0.11	0/1801	0.32	0/2440
2	f	0.11	0/1832	0.36	1/2481 (0.0%)
3	N	0.11	0/1966	0.33	0/2648
3	g	0.12	0/1966	0.36	0/2648
4	O	0.14	0/1851	0.44	2/2501 (0.1%)
4	a	0.12	0/1851	0.40	1/2501 (0.0%)
5	P	0.12	0/1818	0.34	0/2455
5	b	0.10	0/1818	0.35	1/2455 (0.0%)
6	Q	0.11	0/1880	0.34	0/2541
6	c	0.12	0/1880	0.40	1/2541 (0.0%)
7	R	0.10	0/1914	0.31	0/2578
7	d	0.11	0/1914	0.34	0/2578
8	A	0.10	0/1714	0.28	0/2315
8	D	0.11	0/1708	0.32	0/2308
8	F	0.12	0/1726	0.32	0/2331
9	B	0.13	0/1751	0.32	0/2366
9	C	0.11	0/1692	0.34	0/2285
9	E	0.13	0/1713	0.34	0/2309
9	G	0.12	0/1681	0.35	0/2267
10	H	0.13	0/1623	0.44	0/2188
10	S	0.14	0/1623	0.41	0/2188
11	I	0.12	0/1627	0.38	1/2201 (0.0%)
11	T	0.11	0/1618	0.35	0/2190
12	J	0.12	0/1676	0.38	0/2258
12	U	0.13	0/1676	0.39	0/2258
13	K	0.12	0/1718	0.38	0/2324
13	V	0.15	0/1715	0.44	0/2319
14	W	0.12	0/1529	0.35	0/2071
14	Z	0.11	0/1529	0.33	0/2071
15	1	0.15	0/1637	0.42	0/2225
15	X	0.14	0/1637	0.40	0/2225
16	2	0.12	0/1592	0.38	0/2145

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	Y	0.13	0/1592	0.36	0/2145
All	All	0.12	0/61042	0.36	7/82460 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	c	78	THR	N-CA-C	7.16	120.13	111.82
5	b	187	LYS	CB-CA-C	-6.45	109.13	116.54
4	a	213	ARG	CB-CA-C	-5.54	110.17	116.54
2	f	41	ALA	CB-CA-C	-5.47	109.79	117.23
11	I	24	ASN	CB-CA-C	-5.27	110.52	116.63
4	O	215	GLN	CA-C-N	5.09	125.30	120.31
4	O	215	GLN	C-N-CA	5.09	125.30	120.31

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1850	0	1859	36	0
1	e	1856	0	1866	35	0
2	M	1763	0	1759	26	0
2	f	1793	0	1787	29	0
3	N	1936	0	1961	61	0
3	g	1936	0	1961	37	0
4	O	1824	0	1851	52	0
4	a	1824	0	1851	42	0
5	P	1790	0	1773	32	0
5	b	1790	0	1773	51	0
6	Q	1846	0	1832	23	0
6	c	1846	0	1832	48	0
7	R	1879	0	1864	37	0
7	d	1879	0	1864	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1684	0	1721	31	0
8	D	1678	0	1713	62	0
8	F	1695	0	1733	36	0
9	B	1720	0	1759	24	0
9	C	1663	0	1700	26	0
9	E	1685	0	1725	23	0
9	G	1654	0	1698	40	0
10	H	1594	0	1613	61	0
10	S	1594	0	1613	52	0
11	I	1593	0	1597	40	0
11	T	1584	0	1584	31	0
12	J	1645	0	1644	44	0
12	U	1645	0	1644	52	0
13	K	1685	0	1665	59	0
13	V	1682	0	1661	77	0
14	W	1500	0	1459	36	0
14	Z	1500	0	1459	46	0
15	1	1611	0	1624	30	0
15	X	1611	0	1624	47	0
16	2	1561	0	1516	43	0
16	Y	1561	0	1516	37	0
All	All	59957	0	60101	1214	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:25:MET:CE	8:D:236:PRO:HG3	1.51	1.40
12:U:69:PRO:HG3	12:U:222:LYS:NZ	1.34	1.38
3:N:25:MET:HE1	8:D:236:PRO:CG	1.61	1.30
10:H:140:GLY:O	10:H:143:THR:HG23	1.52	1.09
15:X:60:THR:HG22	15:X:65:VAL:HA	1.13	1.07
13:K:59:LEU:HD13	13:K:181:SER:HB3	1.32	1.06
3:N:25:MET:HE1	8:D:236:PRO:CB	1.88	1.03
12:U:69:PRO:CG	12:U:222:LYS:NZ	2.22	1.02
12:U:69:PRO:CG	12:U:222:LYS:HZ2	1.73	1.01
3:N:25:MET:HE1	8:D:236:PRO:HG3	1.02	1.00
13:V:50:MET:HE3	14:Z:136:SER:CB	1.91	1.00
8:D:136:ASN:HD22	8:D:231:LYS:HE3	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:76:LEU:HG	8:D:239:TYR:HB3	1.42	0.98
3:N:155:ASN:HD22	8:D:238:MET:CG	1.79	0.94
11:T:87:ASN:O	11:T:91:TYR:HD2	1.52	0.92
13:V:50:MET:HE3	14:Z:136:SER:HB3	1.50	0.91
13:K:59:LEU:CD1	13:K:181:SER:HB3	2.01	0.90
15:X:60:THR:HG22	15:X:65:VAL:CA	1.98	0.90
3:N:155:ASN:ND2	8:D:238:MET:CG	2.35	0.89
3:N:25:MET:SD	8:D:236:PRO:HG3	2.13	0.87
3:N:155:ASN:ND2	8:D:238:MET:HG3	1.89	0.86
3:N:155:ASN:HD22	8:D:238:MET:CB	1.88	0.86
13:V:50:MET:HG2	14:Z:136:SER:HB3	1.58	0.86
4:O:146:GLN:HE22	9:E:247:MET:HE1	1.42	0.85
3:N:1:MET:HG2	7:R:127:SER:OG	1.75	0.85
4:O:146:GLN:NE2	9:E:247:MET:HE1	1.93	0.84
4:O:76:LEU:HA	8:D:239:TYR:CB	2.08	0.83
3:N:25:MET:CE	8:D:236:PRO:CG	2.37	0.81
4:a:215:GLN:OE1	4:a:216:PRO:HD2	1.80	0.81
11:I:29:LYS:HE3	11:I:31:ASP:HB2	1.62	0.81
15:1:233:LYS:H	15:1:234:PRO:HD3	1.46	0.81
13:V:50:MET:CE	14:Z:136:SER:O	2.29	0.81
13:K:59:LEU:HD13	13:K:181:SER:CB	2.09	0.80
13:V:50:MET:CE	14:Z:136:SER:HB3	2.12	0.80
14:Z:21:THR:N	14:Z:189:SER:HG	1.79	0.80
13:K:59:LEU:HD11	13:K:199:LEU:HD21	1.64	0.79
13:V:51:VAL:HG11	14:Z:138:MET:SD	2.22	0.79
8:D:136:ASN:ND2	8:D:231:LYS:HE3	1.97	0.78
4:O:76:LEU:HG	8:D:239:TYR:CB	2.14	0.78
10:S:143:THR:HG23	10:S:144:GLU:N	1.99	0.78
12:U:69:PRO:HG3	12:U:222:LYS:HZ3	1.44	0.77
11:T:13:VAL:HG23	11:T:113:PRO:HB2	1.66	0.77
10:H:140:GLY:O	10:H:143:THR:CG2	2.33	0.77
15:X:60:THR:CG2	15:X:65:VAL:HA	2.06	0.77
7:d:144:ASN:HD21	14:W:126:ARG:HD2	1.48	0.76
13:K:72:LEU:HD22	13:K:229:TYR:HB2	1.67	0.76
14:W:195:LEU:HB2	14:W:206:ARG:HB2	1.66	0.76
7:R:111:HIS:HB2	14:Z:90:LEU:HD21	1.69	0.75
1:e:70:PHE:HB2	1:e:78:CYS:HB3	1.69	0.75
8:D:237:SER:O	8:D:239:TYR:CD2	2.40	0.75
15:1:233:LYS:N	15:1:234:PRO:HD3	2.01	0.74
12:U:164:LYS:NZ	16:2:100:THR:OG1	2.21	0.74
4:a:43:LEU:HD11	4:a:134:VAL:HG21	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:71:ASP:HB3	5:b:74:ILE:HB	1.69	0.73
10:H:176:ASP:OD2	12:U:185:ASN:ND2	2.22	0.73
13:V:50:MET:SD	14:Z:136:SER:HB3	2.29	0.73
7:d:68:PHE:HB2	7:d:76:MET:HB3	1.69	0.72
7:d:101:SER:O	13:K:110:GLN:NE2	2.22	0.72
13:V:50:MET:CG	14:Z:136:SER:HB3	2.18	0.72
12:U:66:ARG:HH22	15:X:203:LEU:HB3	1.54	0.72
10:H:58:THR:O	11:I:85:ARG:NH2	2.23	0.72
13:K:59:LEU:HD22	13:K:195:LEU:HD22	1.72	0.72
1:e:93:ARG:HE	1:e:121:ILE:HD13	1.55	0.72
14:Z:64:ALA:HB3	14:Z:119:MET:HB3	1.72	0.72
5:b:13:ASN:HB3	6:c:126:ARG:HB3	1.72	0.71
6:Q:72:ILE:HD11	6:Q:132:LEU:HB3	1.72	0.71
10:H:29:GLY:HA3	10:H:34:MET:HA	1.72	0.71
2:M:77:SER:HB3	2:M:163:MET:HE2	1.72	0.71
10:H:127:ILE:HD12	15:X:89:ALA:H	1.55	0.71
7:d:9:ASP:O	7:d:23:GLN:NE2	2.22	0.71
9:C:117:LEU:HD22	9:C:212:ILE:HG23	1.73	0.71
13:V:59:LEU:HD12	13:V:180:PRO:O	1.91	0.70
15:1:60:THR:HG22	15:1:65:VAL:HA	1.73	0.70
9:G:149:GLY:HA2	9:G:236:LYS:HG2	1.74	0.70
15:1:233:LYS:N	15:1:234:PRO:CD	2.54	0.70
7:d:190:VAL:HG12	7:d:194:VAL:HG23	1.71	0.70
10:S:22:ILE:HD11	10:S:110:ALA:HB3	1.73	0.70
12:U:69:PRO:HG3	12:U:222:LYS:HZ2	0.77	0.70
4:O:76:LEU:HA	8:D:239:TYR:CA	2.23	0.69
8:A:170:GLU:HB3	8:A:194:ARG:HE	1.57	0.69
15:1:212:VAL:HB	15:1:229:SER:HB3	1.75	0.69
2:M:136:ILE:HB	2:M:147:PHE:HB2	1.74	0.69
3:N:11:ILE:HA	4:O:18:GLN:HE22	1.57	0.69
10:S:27:ARG:NH2	10:S:205:ASP:OXT	2.26	0.69
4:O:76:LEU:HA	8:D:239:TYR:HB2	1.76	0.68
13:V:50:MET:HE2	13:V:103:ALA:CB	2.24	0.68
7:R:48:PHE:HB2	7:R:215:SER:HB3	1.76	0.68
12:U:215:VAL:HB	15:X:206:LEU:HB3	1.76	0.68
13:V:50:MET:HG2	14:Z:136:SER:CB	2.23	0.68
1:L:12:HIS:O	1:L:24:GLN:NE2	2.26	0.68
6:c:155:ASP:HB3	7:d:63:SER:HB2	1.75	0.68
3:g:90:LEU:HD21	3:g:114:LEU:HD22	1.76	0.68
1:L:24:GLN:HE22	7:R:14:THR:HA	1.58	0.68
15:1:114:ARG:HH12	15:1:144:PHE:HB3	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:55:THR:HB	12:U:68:SER:H	1.59	0.68
13:V:50:MET:HE3	14:Z:136:SER:C	2.19	0.68
3:g:62:SER:HB2	3:g:65:ILE:HB	1.75	0.68
10:H:70:ARG:CD	10:H:90:MET:HE1	2.24	0.68
10:H:149:MET:HE1	12:U:179:ASN:HD22	1.59	0.67
10:H:140:GLY:C	10:H:143:THR:HG23	2.19	0.67
7:R:124:THR:HG22	7:R:131:PRO:HB3	1.77	0.67
13:V:52:THR:HG23	13:V:152:TRP:CZ3	2.28	0.67
13:V:82:ARG:NH1	14:W:218:ASP:O	2.25	0.67
3:N:30:HIS:O	3:N:50:ARG:NH1	2.26	0.67
3:N:48:GLU:HG3	3:N:197:LEU:HD22	1.77	0.67
13:V:237:VAL:HG22	13:V:242:VAL:HG22	1.77	0.67
3:N:155:ASN:HD22	8:D:238:MET:HG3	1.49	0.67
3:g:72:MET:HG2	3:g:138:GLY:HA3	1.78	0.66
9:B:28:LEU:HA	9:B:32:TYR:HB3	1.77	0.66
10:S:27:ARG:HH21	10:S:183:MET:HG3	1.60	0.66
10:S:143:THR:CG2	10:S:144:GLU:N	2.59	0.66
13:V:88:MET:HB2	13:V:109:LYS:HE3	1.76	0.66
15:X:61:ASN:HD21	15:X:66:ALA:HB2	1.60	0.66
11:I:13:VAL:HG23	11:I:113:PRO:HB2	1.76	0.66
3:N:25:MET:SD	8:D:236:PRO:CG	2.82	0.66
1:e:61:LEU:HD11	1:e:66:VAL:HG21	1.77	0.66
6:Q:7:ASP:O	6:Q:21:GLN:NE2	2.29	0.65
1:e:38:THR:HA	1:e:169:GLY:HA3	1.78	0.65
4:O:76:LEU:HA	8:D:239:TYR:HA	1.79	0.65
9:B:41:ASP:HA	9:B:220:ARG:HH11	1.61	0.65
11:I:87:ASN:O	11:I:91:TYR:CD2	2.49	0.65
11:I:102:LEU:HD11	11:I:118:MET:HE3	1.77	0.65
7:d:72:ARG:HB3	7:d:100:ARG:HH22	1.62	0.65
1:L:70:PHE:HD2	1:L:91:VAL:HG21	1.61	0.65
12:U:236:VAL:HG13	12:U:237:PRO:HD2	1.79	0.65
16:Y:155:LEU:HD23	16:Y:186:VAL:HG21	1.78	0.65
8:A:190:LEU:HD12	9:C:178:PHE:HB2	1.77	0.65
2:f:22:ILE:HG21	2:f:152:SER:HB3	1.79	0.65
2:f:43:GLY:CA	2:f:184:LEU:HD21	2.27	0.65
2:M:39:LYS:NZ	3:N:57:ASP:OD2	2.30	0.65
3:N:136:TYR:HB2	3:N:148:TYR:HB2	1.78	0.65
12:J:158:TYR:OH	16:Y:129:ARG:NH2	2.29	0.65
13:K:52:THR:OG1	13:K:227:ARG:NH2	2.27	0.65
16:Y:100:THR:HG22	16:Y:102:LYS:H	1.62	0.65
15:1:46:VAL:HG22	15:1:51:VAL:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:4:ASN:OD1	9:G:146:ASN:ND2	2.30	0.64
8:D:231:LYS:C	8:D:233:GLU:H	2.05	0.64
2:f:70:LYS:HE3	2:f:219:ARG:HH22	1.63	0.64
7:R:9:ASP:HB3	7:R:22:PHE:HD2	1.62	0.64
14:Z:77:ASP:OD2	15:1:123:ARG:NH2	2.30	0.64
4:O:86:ARG:NH1	4:O:118:TYR:OH	2.30	0.64
6:c:146:GLN:HE22	6:c:161:ILE:HG21	1.63	0.64
10:H:7:ASN:HD22	10:H:57:ALA:H	1.43	0.64
10:H:140:GLY:N	10:H:143:THR:CG2	2.61	0.64
9:E:147:ASN:OD1	9:E:150:VAL:HB	1.97	0.64
9:G:239:LYS:N	9:G:240:PRO:CD	2.61	0.64
6:Q:205:LEU:HG	6:Q:210:VAL:HG21	1.80	0.63
15:X:191:GLN:HE21	15:X:216:VAL:HG21	1.62	0.63
6:Q:50:LYS:HB3	6:Q:59:HIS:HB3	1.81	0.63
2:f:19:LEU:HD13	2:f:22:ILE:HD12	1.79	0.63
14:Z:97:LEU:O	14:Z:101:ASN:ND2	2.30	0.63
8:F:9:LEU:HD23	8:F:14:ARG:HD3	1.81	0.63
13:V:50:MET:HE3	14:Z:136:SER:HB2	1.79	0.63
6:c:74:ILE:HD13	6:c:81:ALA:HB2	1.80	0.63
14:Z:104:ARG:HD3	14:Z:139:LEU:HB2	1.81	0.63
11:I:37:LYS:O	11:I:61:GLN:NE2	2.32	0.63
7:d:171:GLN:HA	7:d:174:LYS:HB2	1.81	0.63
4:O:6:ALA:HB2	5:P:125:GLU:HG2	1.80	0.63
6:c:43:HIS:HA	6:c:216:GLY:HA2	1.81	0.62
12:J:153:ASP:OD1	12:J:157:SER:N	2.32	0.62
12:U:127:ARG:NH1	12:U:132:TYR:OH	2.32	0.62
16:2:90:SER:OG	16:2:247:ASN:ND2	2.30	0.62
5:b:79:SER:HB3	5:b:140:ALA:HB3	1.82	0.62
2:f:136:ILE:HB	2:f:147:PHE:HB2	1.82	0.62
13:V:101:ASP:O	13:V:153:ASN:ND2	2.31	0.62
13:V:224:ARG:HH12	14:W:48:ASN:HA	1.64	0.62
16:2:236:THR:HG22	16:2:242:SER:HB3	1.79	0.62
3:N:6:ASP:OD2	4:O:5:ARG:NH1	2.33	0.62
7:R:16:SER:HB3	7:R:20:ARG:H	1.64	0.62
2:f:34:PRO:HA	2:f:164:GLY:HA3	1.81	0.62
2:f:205:GLU:HB3	2:f:230:LEU:HD11	1.81	0.62
13:V:108:LEU:HD23	13:V:155:MET:HE1	1.82	0.62
5:b:173:ALA:HB1	5:b:205:VAL:HB	1.82	0.62
11:I:171:PHE:O	11:T:174:ASN:ND2	2.32	0.62
1:L:132:ARG:HD3	7:R:13:SER:HA	1.82	0.62
16:2:91:ARG:NH2	16:2:240:SER:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:38:MET:HA	11:I:61:GLN:HG3	1.80	0.62
11:I:38:MET:O	11:I:65:GLN:NE2	2.31	0.62
12:J:236:VAL:HG13	12:J:237:PRO:HD2	1.82	0.62
2:M:119:GLN:NE2	3:N:81:SER:O	2.32	0.61
6:c:11:THR:HA	7:d:130:ARG:HD3	1.80	0.61
13:K:54:THR:HG22	13:K:86:ARG:HH12	1.65	0.61
12:U:103:TYR:CE1	12:U:107:ASN:OD1	2.53	0.61
12:J:50:ILE:HG12	12:J:225:ILE:HG12	1.81	0.61
6:c:229:VAL:HG12	6:c:233:LEU:HG	1.82	0.61
10:S:204:MET:HB2	16:Y:268:MET:HG3	1.83	0.61
12:U:55:THR:HG21	12:U:222:LYS:HE3	1.81	0.61
16:Y:100:THR:HB	16:Y:103:VAL:HG23	1.83	0.61
10:H:2:SER:N	10:H:5:SER:HG	1.98	0.61
12:J:181:VAL:HG22	12:J:194:LEU:HD22	1.82	0.61
16:Y:106:VAL:HG13	16:Y:114:LEU:HD21	1.81	0.61
14:Z:23:ILE:HD11	14:Z:135:MET:HE1	1.82	0.61
7:R:55:LEU:HB2	7:R:59:TYR:HE2	1.65	0.61
4:a:212:ARG:O	4:a:215:GLN:HB2	2.00	0.61
2:f:43:GLY:N	2:f:184:LEU:HD21	2.15	0.61
15:X:61:ASN:ND2	15:X:66:ALA:HB2	2.16	0.61
1:L:187:PHE:HZ	1:L:193:GLN:HG3	1.65	0.61
7:d:214:LEU:HB2	7:d:228:VAL:HG11	1.82	0.61
13:V:72:LEU:HD22	13:V:229:TYR:HB2	1.82	0.61
15:X:67:ASP:HB3	15:X:70:CYS:HB2	1.83	0.60
8:A:64:LEU:HD13	8:A:94:LEU:HB3	1.82	0.60
2:f:65:VAL:HG22	2:f:75:VAL:HG12	1.83	0.60
13:V:91:ASN:ND2	13:V:127:SER:OG	2.34	0.60
10:H:70:ARG:HD3	10:H:90:MET:HE1	1.83	0.60
10:H:113:ASP:N	10:H:118:LYS:O	2.32	0.60
13:V:50:MET:HE1	14:Z:136:SER:O	1.99	0.60
3:N:216:LEU:HD12	3:N:225:ILE:HD12	1.82	0.60
7:d:66:ARG:NH2	7:d:78:VAL:O	2.30	0.60
13:V:51:VAL:HG23	13:V:51:VAL:O	2.01	0.60
9:B:118:LYS:NZ	8:D:193:GLU:OE1	2.33	0.60
12:J:38:GLY:HA3	12:J:70:LYS:HE2	1.84	0.60
13:K:73:GLY:N	13:K:81:PHE:O	2.34	0.60
11:T:87:ASN:O	11:T:91:TYR:CD2	2.44	0.60
3:N:25:MET:HE1	8:D:236:PRO:HB3	1.78	0.60
4:O:50:VAL:HG11	4:O:54:GLN:H	1.65	0.60
7:R:9:ASP:O	7:R:23:GLN:NE2	2.34	0.60
10:S:27:ARG:NH1	10:S:179:ALA:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:237:SER:C	8:D:238:MET:HE3	2.26	0.59
12:J:55:THR:HB	12:J:67:ASP:HA	1.84	0.59
16:2:79:LYS:N	16:2:196:ASN:O	2.32	0.59
11:T:168:GLN:NE2	11:T:174:ASN:O	2.34	0.59
12:U:69:PRO:CG	12:U:222:LYS:HZ3	2.05	0.59
9:C:44:LEU:HA	9:C:49:LEU:HD23	1.84	0.59
9:G:15:ASP:OD1	9:G:18:ARG:NH2	2.35	0.59
13:K:130:PRO:HD2	13:K:161:ALA:HB2	1.84	0.59
3:N:62:SER:OG	3:N:65:ILE:O	2.20	0.59
8:F:7:VAL:HG12	9:G:26:GLU:HG2	1.84	0.59
3:g:49:ARG:NH2	3:g:63:GLU:OE1	2.36	0.59
8:F:64:LEU:HD11	8:F:175:VAL:HG22	1.83	0.59
4:a:42:VAL:HA	4:a:210:VAL:HG12	1.84	0.59
2:f:86:LEU:HD13	2:f:134:LEU:HD11	1.84	0.59
15:X:40:THR:N	15:X:207:GLY:O	2.36	0.59
3:N:50:ARG:HD3	9:B:248:ILE:HG23	1.85	0.59
3:g:73:ALA:HB2	3:g:225:ILE:HD13	1.85	0.59
14:Z:217:TYR:CZ	14:Z:219:GLU:HB3	2.37	0.59
3:N:140:ASP:OD1	3:N:144:GLY:N	2.35	0.59
12:J:44:ALA:HB2	12:J:149:VAL:HG23	1.84	0.59
12:J:85:PHE:HZ	13:K:173:LEU:HB3	1.67	0.59
1:L:85:ALA:HB2	7:R:155:SER:HB2	1.85	0.58
4:a:195:LEU:HD13	4:a:206:ILE:HD13	1.85	0.58
6:c:39:LYS:HE2	6:c:157:ARG:HA	1.84	0.58
10:S:113:ASP:N	10:S:118:LYS:O	2.33	0.58
11:T:38:MET:O	11:T:65:GLN:NE2	2.36	0.58
12:U:44:ALA:HB2	12:U:149:VAL:HG23	1.84	0.58
12:U:212:GLU:HG2	12:U:239:ARG:HH11	1.68	0.58
5:P:90:ASP:OD1	5:P:93:ARG:NH2	2.36	0.58
12:J:120:LEU:HD23	12:J:152:PHE:HE2	1.67	0.58
8:F:114:LEU:HD22	8:F:157:VAL:HG21	1.84	0.58
5:b:20:ARG:HH22	6:c:31:GLN:HB3	1.67	0.58
4:a:137:ASP:HB2	4:a:141:THR:HB	1.85	0.58
11:I:145:ARG:HG3	16:2:230:ARG:HD3	1.85	0.58
13:V:52:THR:HG23	13:V:152:TRP:HZ3	1.67	0.58
15:X:75:PHE:HD1	15:X:81:TYR:HE1	1.51	0.58
3:N:70:GLU:OE2	3:N:222:LYS:NZ	2.35	0.58
9:E:18:ARG:HE	9:E:137:LEU:HB3	1.68	0.58
7:d:85:ALA:O	7:d:89:ALA:N	2.37	0.58
10:S:143:THR:CG2	10:S:144:GLU:H	2.16	0.58
11:T:181:ARG:HD3	11:T:188:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:7:VAL:HG11	9:B:29:LEU:HD12	1.85	0.58
11:I:170:ARG:NH1	11:T:27:GLN:O	2.35	0.58
13:K:96:LEU:HG	13:K:157:ILE:HG12	1.84	0.58
10:S:99:ARG:O	10:S:102:PRO:HG3	2.03	0.58
9:B:57:LEU:O	9:B:107:ASN:ND2	2.36	0.58
8:D:20:PHE:HA	8:D:24:LEU:HB3	1.86	0.58
9:G:44:LEU:HA	9:G:49:LEU:HD12	1.86	0.58
9:G:206:GLU:HB3	9:G:210:ARG:HH12	1.69	0.58
4:a:120:GLN:HG3	5:b:135:ARG:HG2	1.83	0.58
7:d:151:MET:HB3	7:d:161:TYR:HE2	1.69	0.58
10:S:189:ILE:HB	10:S:196:THR:HB	1.85	0.58
14:W:197:THR:HB	14:W:204:ASP:HB2	1.86	0.58
10:S:155:GLU:OE2	15:1:242:ARG:NH2	2.37	0.58
1:L:193:GLN:NE2	1:L:196:GLU:OE1	2.36	0.58
12:J:97:GLU:HA	12:J:100:LEU:HD12	1.86	0.58
13:V:144:ARG:HB3	13:V:150:PRO:HA	1.85	0.58
15:X:46:VAL:HG22	15:X:51:VAL:HG12	1.85	0.58
8:A:43:LEU:HD23	8:A:46:LEU:HD12	1.86	0.57
13:V:54:THR:HG21	13:V:70:ASP:HB2	1.86	0.57
3:N:1:MET:CE	7:R:128:ALA:HB2	2.33	0.57
8:D:52:LEU:O	8:D:203:ARG:NH1	2.38	0.57
8:D:237:SER:O	8:D:238:MET:HE3	2.03	0.57
8:F:132:ILE:HD13	9:G:152:VAL:HG11	1.85	0.57
8:A:61:ARG:HD2	8:A:192:HIS:HB3	1.86	0.57
2:f:179:ASN:OD1	2:f:180:GLU:N	2.34	0.57
10:H:84:PRO:HD3	10:H:114:PRO:HD3	1.85	0.57
2:M:124:SER:HA	3:N:127:LYS:HE2	1.85	0.57
16:2:75:THR:HA	16:2:88:VAL:HG12	1.86	0.57
3:N:155:ASN:HD22	8:D:238:MET:HB2	1.65	0.57
10:H:169:GLN:O	10:H:173:ASN:ND2	2.34	0.57
14:Z:39:ARG:NH1	14:Z:187:GLY:O	2.37	0.57
10:H:70:ARG:HD2	10:H:90:MET:HE1	1.85	0.57
12:J:35:PHE:HZ	12:J:168:SER:HB3	1.69	0.57
12:U:153:ASP:OD1	12:U:157:SER:N	2.38	0.57
14:W:28:PHE:HE2	14:W:33:VAL:HG23	1.70	0.57
11:I:4:LEU:HB2	11:I:132:HIS:HD2	1.70	0.57
14:W:34:VAL:HB	14:W:196:ALA:HB3	1.86	0.57
1:L:38:THR:HG21	1:L:171:LYS:HB2	1.86	0.56
9:G:241:ARG:HG2	9:G:241:ARG:O	2.04	0.56
13:K:104:ASP:OD1	14:W:111:ARG:NH1	2.34	0.56
10:H:113:ASP:HB2	10:H:118:LYS:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Y:249:TYR:HE1	16:Y:258:LYS:HG3	1.70	0.56
3:N:4:ARG:NH1	5:P:9:ASP:OD1	2.38	0.56
3:N:184:MET:HE2	3:N:189:ALA:HA	1.87	0.56
13:V:50:MET:HE2	13:V:103:ALA:HB2	1.87	0.56
6:c:45:VAL:HG22	6:c:214:ILE:HG12	1.86	0.56
10:H:49:LEU:HD21	10:H:87:LEU:HD22	1.88	0.56
13:K:72:LEU:HD11	13:K:79:ALA:HB1	1.87	0.56
16:Y:226:ASP:OD1	16:Y:229:ARG:NH2	2.38	0.56
2:M:19:LEU:HD13	2:M:22:ILE:HD12	1.88	0.56
3:N:166:ASN:OD1	3:N:167:ASN:N	2.38	0.56
1:e:32:ILE:HD13	1:e:137:CYS:HB2	1.87	0.56
1:e:153:LYS:HB3	1:e:163:PHE:HE2	1.70	0.56
13:K:196:ARG:NH1	15:1:203:LEU:O	2.38	0.56
3:g:140:ASP:OD1	3:g:144:GLY:N	2.39	0.56
10:H:37:THR:HG22	10:H:183:MET:HB3	1.88	0.56
8:D:237:SER:C	8:D:239:TYR:H	2.13	0.56
4:a:115:LYS:HG2	4:a:127:PHE:HD2	1.70	0.56
13:V:219:ARG:HG3	13:V:252:THR:HG22	1.86	0.56
10:H:29:GLY:HA2	10:H:35:VAL:HG23	1.88	0.56
15:X:45:LEU:HD11	15:X:190:ALA:HB1	1.88	0.56
16:Y:73:THR:N	16:Y:241:TYR:O	2.39	0.56
1:L:123:GLN:HE22	2:M:84:ARG:HB2	1.71	0.56
2:M:65:VAL:HG22	2:M:75:VAL:HG12	1.86	0.56
8:D:237:SER:O	8:D:239:TYR:N	2.36	0.55
8:F:185:MET:HA	8:F:188:ARG:HE	1.70	0.55
1:e:163:PHE:HD2	1:e:166:THR:HG22	1.71	0.55
15:X:84:GLY:HA2	15:X:137:LEU:HD23	1.88	0.55
5:P:211:ASN:OD1	5:P:212:ALA:N	2.40	0.55
10:H:34:MET:HE1	10:H:183:MET:HE2	1.87	0.55
16:Y:75:THR:HG23	16:Y:88:VAL:HG12	1.87	0.55
8:D:136:ASN:HD22	8:D:231:LYS:CE	2.08	0.55
2:M:74:LEU:HD13	2:M:134:LEU:HD23	1.88	0.55
4:O:92:GLN:HG3	11:T:66:LEU:HB2	1.89	0.55
8:D:163:THR:HA	8:D:166:LYS:HD3	1.88	0.55
2:M:69:THR:HG22	2:M:72:ILE:HB	1.89	0.55
3:N:155:ASN:ND2	8:D:238:MET:O	2.40	0.55
5:b:183:GLU:O	5:b:186:HIS:NE2	2.39	0.55
6:c:33:SER:HB2	6:c:51:ARG:HD2	1.89	0.55
12:U:64:HIS:O	13:V:196:ARG:NH2	2.39	0.55
16:2:216:ARG:HE	16:2:220:SER:H	1.52	0.55
8:A:64:LEU:HB3	8:A:94:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:41:GLN:NE2	5:b:151:PRO:O	2.40	0.55
10:S:88:MET:HG3	10:S:124:LEU:HD11	1.89	0.55
10:S:83:LYS:HA	10:S:114:PRO:HG3	1.88	0.55
5:b:182:GLN:HA	6:c:56:LEU:HD21	1.88	0.55
13:K:80:ARG:NH1	14:W:135:MET:SD	2.76	0.55
10:S:96:TYR:HA	10:S:99:ARG:HB2	1.88	0.55
3:N:180:LYS:HD3	3:N:184:MET:HB2	1.89	0.55
4:O:181:ILE:HG22	4:O:187:THR:HG23	1.88	0.55
9:B:188:ALA:HA	9:B:197:TYR:HB3	1.89	0.55
9:C:181:ARG:HG3	9:C:201:VAL:HG13	1.89	0.55
11:I:101:ASN:HB3	11:I:132:HIS:ND1	2.21	0.55
2:M:102:GLN:OE1	15:1:96:ARG:NH1	2.41	0.55
7:d:234:GLU:HA	7:d:237:GLU:HB2	1.89	0.55
1:e:113:MET:HG3	15:X:109:THR:HG22	1.88	0.55
10:H:205:ASP:OD2	16:2:91:ARG:NH1	2.40	0.55
12:J:41:LEU:HD11	12:J:177:LEU:HD11	1.87	0.55
12:J:86:HIS:HD2	13:K:175:VAL:HG13	1.70	0.55
15:X:54:GLY:HA3	15:X:194:LEU:HD11	1.89	0.55
15:X:77:ALA:HB3	15:X:80:ILE:HB	1.88	0.55
9:C:114:LEU:HB3	9:C:118:LYS:HE3	1.89	0.54
11:I:87:ASN:O	11:I:91:TYR:HD2	1.90	0.54
10:H:127:ILE:HB	15:X:89:ALA:HB3	1.89	0.54
3:N:28:ILE:HD13	3:N:133:SER:HB2	1.89	0.54
2:f:45:VAL:HA	2:f:212:ILE:HG22	1.89	0.54
10:H:105:THR:HG23	10:H:107:PRO:HD3	1.89	0.54
12:U:66:ARG:NH2	15:X:203:LEU:HB3	2.23	0.54
16:2:155:LEU:HD23	16:2:186:VAL:HG21	1.89	0.54
2:M:122:THR:HG22	2:M:129:PRO:HB3	1.89	0.54
5:b:161:THR:OG1	6:c:78:THR:OG1	2.20	0.54
1:L:51:VAL:HG22	1:L:217:VAL:HG22	1.89	0.54
4:a:11:SER:OG	4:a:15:HIS:N	2.41	0.54
7:d:50:VAL:HG11	7:d:66:ARG:HB2	1.90	0.54
4:a:120:GLN:NE2	5:b:135:ARG:O	2.35	0.54
6:c:129:GLY:HA2	6:c:149:PRO:HB3	1.89	0.54
1:e:71:LYS:HG2	14:W:88:MET:HE1	1.88	0.54
14:W:118:LEU:O	14:W:134:THR:OG1	2.23	0.54
8:D:238:MET:HG2	8:D:239:TYR:N	2.22	0.54
9:G:238:LYS:HB2	9:G:240:PRO:HD2	1.89	0.54
12:U:136:ASN:HB2	12:U:152:PHE:HB2	1.88	0.54
4:O:154:HIS:HD1	5:P:64:ILE:HD11	1.73	0.54
8:D:130:PRO:HD3	8:D:230:PRO:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:207:THR:HB	6:c:226:ASP:HB2	1.89	0.54
10:S:143:THR:HG23	10:S:144:GLU:H	1.71	0.54
9:C:22:CYS:SG	9:C:134:TRP:NE1	2.72	0.54
4:a:5:ARG:NE	3:g:6:ASP:OD2	2.41	0.54
4:a:115:LYS:HG2	4:a:127:PHE:CD2	2.43	0.54
5:b:211:ASN:HB2	5:b:214:ASN:HB2	1.89	0.54
14:W:124:ASP:OD1	14:W:128:GLY:N	2.41	0.54
5:P:110:GLU:HA	5:P:154:PHE:HE2	1.73	0.54
6:Q:49:LEU:HB2	6:Q:195:LEU:HD11	1.90	0.54
8:F:17:VAL:O	8:F:21:ARG:N	2.39	0.54
1:e:144:ASP:O	1:e:148:GLY:N	2.39	0.54
1:e:155:ASP:OD1	1:e:159:TYR:N	2.41	0.54
3:g:30:HIS:O	3:g:50:ARG:NH1	2.40	0.54
6:c:103:LEU:HD12	6:c:104:PRO:HD2	1.89	0.53
2:f:43:GLY:C	2:f:184:LEU:HD21	2.33	0.53
13:K:181:SER:HB2	13:K:195:LEU:HD13	1.91	0.53
13:V:51:VAL:HG23	13:V:102:TYR:H	1.72	0.53
9:E:245:LYS:HD3	9:E:249:TYR:OH	2.08	0.53
12:J:41:LEU:HD12	12:J:173:LEU:HD13	1.90	0.53
16:Y:80:PHE:HE1	16:Y:82:HIS:HB2	1.73	0.53
1:e:73:THR:HG22	1:e:76:ILE:HB	1.90	0.53
3:g:240:HIS:O	3:g:244:GLU:N	2.42	0.53
9:B:54:LEU:HD23	9:B:206:GLU:HB3	1.89	0.53
7:d:192:LYS:HG2	7:d:236:ALA:HA	1.91	0.53
10:H:106:GLU:OE1	10:H:139:SER:OG	2.25	0.53
10:S:15:LYS:HG3	10:S:20:VAL:HG12	1.89	0.53
10:S:68:LYS:HA	10:S:71:LEU:HB3	1.90	0.53
14:W:27:GLU:OE2	14:W:131:VAL:N	2.37	0.53
13:K:134:HIS:CE1	13:K:176:ALA:HB1	2.44	0.53
1:L:231:THR:HG22	1:L:233:ALA:H	1.73	0.53
12:J:164:LYS:NZ	16:Y:100:THR:OG1	2.26	0.53
11:T:19:ARG:HD3	11:T:177:THR:HG22	1.91	0.53
12:J:159:GLN:HG3	16:Y:103:VAL:HG22	1.90	0.53
8:F:129:ILE:HB	9:G:232:LYS:HE3	1.91	0.53
10:H:153:LEU:HB3	10:H:166:THR:HG23	1.91	0.52
5:P:155:HIS:HB2	5:P:168:ARG:HG3	1.91	0.52
10:H:198:ARG:HG2	15:X:253:GLN:HG2	1.91	0.52
10:S:49:LEU:HD21	10:S:87:LEU:HD22	1.91	0.52
13:V:56:VAL:H	13:V:184:THR:HB	1.74	0.52
14:W:75:ILE:HD11	14:W:114:LEU:HD13	1.91	0.52
16:Y:236:THR:HG22	16:Y:242:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:169:GLU:OE1	14:Z:172:ARG:NH2	2.39	0.52
12:U:30:PHE:HZ	13:V:145:ARG:HG3	1.74	0.52
15:1:142:VAL:HG11	15:1:219:ALA:HA	1.91	0.52
4:O:76:LEU:HD12	8:D:239:TYR:HB2	1.91	0.52
4:O:96:LEU:O	16:2:153:LYS:NZ	2.43	0.52
9:G:117:LEU:HD22	9:G:212:ILE:HG12	1.91	0.52
10:S:61:GLN:NE2	11:T:124:LEU:O	2.39	0.52
16:2:84:VAL:H	16:2:251:MET:HB2	1.74	0.52
4:O:207:GLU:HA	4:O:225:ILE:HD13	1.92	0.52
9:C:41:ASP:OD1	9:C:220:ARG:NH1	2.43	0.52
6:c:39:LYS:HA	6:c:44:ALA:HA	1.91	0.52
3:g:46:ALA:HA	3:g:213:ILE:HG12	1.92	0.52
12:U:83:SER:O	12:U:135:TYR:N	2.33	0.52
8:A:183:HIS:ND1	9:C:102:GLY:O	2.43	0.52
9:G:239:LYS:O	9:G:239:LYS:HG2	2.09	0.52
10:H:99:ARG:O	10:H:102:PRO:HG3	2.09	0.52
13:V:51:VAL:CG2	13:V:102:TYR:HB3	2.39	0.52
5:b:181:LEU:HA	5:b:184:VAL:HG12	1.91	0.52
6:c:9:ASP:HB2	6:c:12:VAL:HG23	1.92	0.52
13:K:59:LEU:HD12	13:K:180:PRO:O	2.09	0.52
12:U:127:ARG:HG3	12:U:132:TYR:CZ	2.45	0.52
2:M:22:ILE:HG21	2:M:152:SER:HB3	1.91	0.52
4:a:146:GLN:HE22	4:a:169:ARG:HH22	1.57	0.52
12:J:66:ARG:NH1	13:K:200:GLU:OE2	2.37	0.52
14:W:157:TYR:HB2	14:Z:156:GLY:HA3	1.90	0.52
16:2:219:LEU:HB3	16:2:224:ALA:HB2	1.91	0.52
8:D:20:PHE:HZ	9:E:41:ASP:HB2	1.75	0.52
8:D:231:LYS:O	8:D:233:GLU:N	2.43	0.52
6:c:13:TRP:HE1	7:d:130:ARG:HB2	1.75	0.52
1:e:123:GLN:NE2	2:f:81:PRO:O	2.43	0.52
10:H:83:LYS:HA	10:H:114:PRO:HG2	1.92	0.52
8:A:114:LEU:HD13	8:A:213:TYR:CE1	2.44	0.51
6:c:72:ILE:HG21	6:c:88:MET:HE1	1.92	0.51
2:f:69:THR:HG23	2:f:71:HIS:H	1.75	0.51
10:S:113:ASP:HB2	10:S:118:LYS:HB3	1.92	0.51
16:2:116:THR:OG1	16:2:172:MET:N	2.42	0.51
5:P:141:LEU:HB2	5:P:156:MET:HB3	1.91	0.51
5:b:168:ARG:HD3	6:c:57:ALA:HB2	1.90	0.51
13:K:134:HIS:HE1	13:K:176:ALA:HB1	1.74	0.51
13:V:116:VAL:HA	13:V:128:TYR:HE2	1.75	0.51
14:Z:179:ILE:HG22	14:Z:183:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:159:ASN:OD1	4:O:160:ALA:N	2.43	0.51
5:P:182:GLN:NE2	6:Q:55:GLU:HB2	2.25	0.51
8:D:238:MET:SD	8:D:239:TYR:HD2	2.33	0.51
5:b:199:LEU:HD23	5:b:202:LEU:HD12	1.93	0.51
6:c:42:THR:HB	6:c:217:LYS:HB2	1.91	0.51
2:M:150:ASP:OD1	2:M:154:ALA:N	2.41	0.51
12:U:236:VAL:CG1	12:U:237:PRO:HD2	2.39	0.51
13:V:105:PHE:HD1	13:V:155:MET:HE2	1.75	0.51
16:Y:197:MET:SD	16:Y:211:MET:HB3	2.51	0.51
3:N:176:LYS:NZ	4:O:51:ALA:HB1	2.26	0.51
4:a:208:LEU:HD12	4:a:225:ILE:HG12	1.91	0.51
7:d:22:PHE:O	7:d:26:TYR:N	2.36	0.51
14:Z:198:ILE:HG12	14:Z:203:VAL:HG22	1.92	0.51
4:a:36:ARG:HA	4:a:41:VAL:HG22	1.92	0.51
4:a:172:LEU:HD21	4:a:194:ALA:HB2	1.92	0.51
3:g:71:ASP:OD2	3:g:104:PRO:HB2	2.10	0.51
10:H:140:GLY:N	10:H:143:THR:HG22	2.24	0.51
5:b:36:THR:HG21	5:b:173:ALA:HB3	1.91	0.51
11:T:8:GLN:HG3	11:T:13:VAL:HG22	1.92	0.51
12:U:88:ASP:OD1	13:V:145:ARG:NH2	2.44	0.51
9:E:104:VAL:HG11	8:F:184:VAL:HG22	1.91	0.51
5:b:86:LYS:HA	5:b:89:ILE:HD12	1.92	0.51
5:b:196:LYS:NZ	5:b:240:ASP:OD2	2.39	0.51
16:Y:93:SER:HA	16:Y:99:ALA:H	1.76	0.51
16:2:199:SER:HB3	16:2:208:TYR:CZ	2.45	0.51
1:L:73:THR:HG22	1:L:76:ILE:HB	1.93	0.51
4:O:77:THR:H	8:D:239:TYR:HA	1.74	0.51
13:V:257:ALA:HA	14:W:50:VAL:HG11	1.93	0.51
2:M:140:ASN:HB2	2:M:145:TYR:HE2	1.76	0.51
4:O:47:LYS:HZ3	4:O:207:GLU:HB3	1.76	0.51
5:b:74:ILE:HG12	5:b:145:GLY:HA3	1.92	0.51
5:b:191:LEU:HD21	5:b:219:THR:HB	1.93	0.51
7:d:93:ARG:HH12	13:K:122:LEU:HD23	1.76	0.51
13:V:134:HIS:HE1	13:V:176:ALA:HB1	1.75	0.51
16:Y:80:PHE:CE1	16:Y:82:HIS:HB2	2.46	0.51
8:F:114:LEU:HD12	8:F:213:TYR:CE2	2.45	0.50
13:K:88:MET:SD	13:K:109:LYS:HG3	2.51	0.50
1:L:153:LYS:HB3	1:L:163:PHE:CE2	2.46	0.50
1:L:171:LYS:HB3	1:L:205:VAL:HG11	1.93	0.50
9:G:59:ALA:HB1	9:G:61:LEU:HD13	1.94	0.50
1:e:211:LYS:HB2	1:e:214:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:77:LYS:HA	12:U:226:VAL:HG11	1.92	0.50
2:M:87:VAL:O	2:M:91:ARG:HG3	2.11	0.50
4:O:180:ALA:O	4:O:181:ILE:HG13	2.11	0.50
4:a:31:THR:HA	4:a:162:GLY:HA3	1.93	0.50
12:J:236:VAL:CG1	12:J:237:PRO:HD2	2.40	0.50
16:2:73:THR:N	16:2:241:TYR:O	2.44	0.50
5:b:97:GLN:HB3	16:Y:133:LYS:HG3	1.93	0.50
10:H:140:GLY:H	10:H:143:THR:CG2	2.24	0.50
13:K:99:SER:HB3	13:K:154:THR:HB	1.93	0.50
1:L:232:GLU:HA	1:L:235:ILE:HD12	1.94	0.50
2:M:34:PRO:HG3	2:M:165:LYS:HB3	1.92	0.50
3:N:1:MET:HE1	7:R:128:ALA:HA	1.92	0.50
8:A:177:LYS:HA	8:A:180:LYS:HE2	1.93	0.50
9:E:106:CYS:HB3	9:E:181:ARG:HH22	1.76	0.50
13:K:52:THR:HG1	13:K:227:ARG:NH2	2.10	0.50
10:S:9:GLY:HA3	10:S:41:LYS:HE2	1.94	0.50
11:T:8:GLN:NE2	11:T:113:PRO:O	2.45	0.50
13:V:52:THR:HG23	13:V:152:TRP:CH2	2.47	0.50
15:X:59:ALA:O	15:X:66:ALA:N	2.41	0.50
8:A:52:LEU:O	8:A:203:ARG:NH1	2.45	0.50
13:K:53:GLY:N	13:K:100:GLY:O	2.44	0.50
14:Z:49:ARG:HG3	14:Z:50:VAL:HG23	1.93	0.50
4:O:37:GLY:HA2	4:O:181:ILE:HB	1.94	0.50
13:K:52:THR:HG1	13:K:227:ARG:HH22	1.53	0.50
13:V:50:MET:CE	14:Z:136:SER:C	2.81	0.50
5:P:113:THR:HG22	5:P:143:PHE:HD2	1.76	0.50
9:G:61:LEU:HD21	9:G:185:VAL:HG22	1.93	0.50
5:b:51:GLU:OE2	5:b:214:ASN:ND2	2.45	0.50
2:f:111:VAL:HG21	2:f:147:PHE:HD2	1.77	0.50
3:g:8:ARG:HB3	3:g:11:ILE:HG12	1.94	0.50
12:J:114:GLY:HA2	12:J:150:TYR:HE2	1.77	0.50
4:O:76:LEU:CG	8:D:239:TYR:CB	2.88	0.50
5:b:113:THR:HG22	5:b:143:PHE:HD2	1.76	0.50
5:b:157:ASP:OD1	5:b:161:THR:N	2.43	0.50
10:H:175:VAL:HG11	10:H:182:GLY:HA2	1.94	0.50
13:K:119:GLU:HB2	13:K:128:TYR:CZ	2.47	0.50
12:U:41:LEU:HD11	12:U:177:LEU:HD21	1.93	0.50
3:N:180:LYS:HB3	3:N:183:GLU:HB2	1.94	0.49
7:R:78:VAL:HG11	7:R:85:ALA:HB1	1.93	0.49
3:g:34:CYS:HB2	3:g:164:ILE:HG13	1.94	0.49
3:g:219:GLU:OE1	3:g:226:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:124:ASP:OD1	14:Z:128:GLY:N	2.40	0.49
7:d:41:ARG:HH11	7:d:148:GLN:HA	1.76	0.49
13:V:82:ARG:NH1	13:V:229:TYR:OH	2.42	0.49
13:V:86:ARG:NH2	13:V:98:ALA:O	2.43	0.49
12:J:185:ASN:ND2	10:S:176:ASP:OD2	2.45	0.49
12:U:41:LEU:HB3	12:U:207:PHE:HZ	1.77	0.49
4:O:209:ALA:HB1	4:O:217:LEU:HD11	1.94	0.49
6:Q:137:TYR:CZ	6:Q:217:LYS:HA	2.48	0.49
9:E:181:ARG:NH2	9:E:205:ASP:OD1	2.43	0.49
8:F:171:ARG:NH1	8:F:195:ASP:OD1	2.45	0.49
11:I:4:LEU:HD22	11:I:45:LEU:HD23	1.94	0.49
12:U:161:ASP:OD1	12:U:162:SER:N	2.45	0.49
1:L:208:ILE:HD12	1:L:210:PHE:HE1	1.78	0.49
13:K:65:VAL:HG23	13:K:165:SER:HB3	1.94	0.49
13:K:141:MET:HE1	13:K:151:LEU:HB2	1.93	0.49
11:T:167:LEU:HA	11:T:171:PHE:HB3	1.94	0.49
3:N:239:LYS:O	3:N:243:GLU:HG3	2.12	0.49
4:a:55:ASP:HB3	3:g:158:GLY:HA3	1.93	0.49
11:I:19:ARG:HD2	11:I:179:SER:HB2	1.95	0.49
13:K:260:ILE:HD11	14:Z:50:VAL:HG12	1.94	0.49
9:B:130:LEU:HD21	8:D:207:LEU:HD11	1.95	0.49
8:D:94:LEU:HD13	9:E:194:VAL:HG22	1.94	0.49
6:c:113:GLY:O	6:c:117:GLN:HG3	2.12	0.49
1:e:47:CYS:HB3	1:e:221:THR:HG22	1.94	0.49
1:e:56:VAL:HA	1:e:61:LEU:HD23	1.95	0.49
11:I:171:PHE:CE2	11:I:173:LEU:HB2	2.47	0.49
13:V:222:TYR:HE2	13:V:250:ALA:HB3	1.78	0.49
15:1:42:ILE:HG13	15:1:138:ILE:HD12	1.94	0.49
15:1:52:ILE:HG12	15:1:216:VAL:HA	1.94	0.49
9:E:7:GLN:HB3	9:E:11:GLN:HG3	1.93	0.49
9:E:161:THR:HA	9:E:164:HIS:HD2	1.78	0.49
5:b:71:ASP:OD1	5:b:72:ALA:N	2.44	0.49
6:c:69:HIS:CD2	6:c:70:ILE:HG13	2.48	0.49
2:f:46:LEU:HD11	2:f:137:CYS:HB2	1.95	0.49
3:g:151:ASP:HB2	3:g:152:PRO:HD2	1.95	0.49
11:I:164:LEU:HB3	11:I:178:PHE:HE2	1.77	0.49
12:J:32:PRO:O	13:K:145:ARG:NH2	2.46	0.49
11:T:116:TYR:HB3	11:T:124:LEU:HD11	1.94	0.49
11:T:171:PHE:CE2	11:T:173:LEU:HB2	2.47	0.49
3:N:1:MET:HE1	7:R:128:ALA:CB	2.43	0.49
5:P:12:VAL:HG13	5:P:23:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:150:VAL:HG22	8:F:216:LEU:HD22	1.95	0.49
4:a:35:VAL:O	4:a:41:VAL:HG13	2.13	0.49
11:I:104:LEU:HD23	11:I:116:TYR:HD2	1.78	0.48
5:P:40:ILE:HG21	5:P:194:ALA:HB1	1.94	0.48
7:R:212:LEU:HD12	7:R:237:GLU:HG2	1.95	0.48
8:A:190:LEU:HD22	8:A:194:ARG:CZ	2.43	0.48
8:F:39:LYS:HE3	8:F:117:LYS:HE3	1.96	0.48
9:G:152:VAL:HB	9:G:236:LYS:HE2	1.96	0.48
6:c:82:ARG:HA	6:c:85:CYS:HB3	1.94	0.48
7:d:93:ARG:NH2	13:K:121:LEU:O	2.46	0.48
11:I:100:VAL:H	11:I:120:TYR:HB3	1.77	0.48
15:1:81:TYR:HB2	15:1:217:ILE:HD11	1.96	0.48
5:P:40:ILE:HB	5:P:47:CYS:HB3	1.94	0.48
6:Q:103:LEU:HD12	6:Q:104:PRO:HD2	1.95	0.48
8:D:128:LEU:HD13	8:D:228:VAL:HA	1.95	0.48
5:b:36:THR:HA	5:b:171:GLY:HA3	1.94	0.48
6:c:8:ASN:HB3	3:g:3:ARG:HH22	1.79	0.48
11:I:18:ASP:O	11:I:34:LYS:NZ	2.32	0.48
16:2:245:VAL:HG12	16:2:263:ASP:HA	1.95	0.48
1:L:92:GLN:NE2	7:R:114:ASP:OD2	2.46	0.48
3:N:1:MET:HE3	7:R:128:ALA:HB2	1.96	0.48
3:N:90:LEU:HG	3:N:114:LEU:HD22	1.95	0.48
10:H:34:MET:O	16:2:238:ARG:NH2	2.46	0.48
1:L:70:PHE:CD2	1:L:91:VAL:HG21	2.46	0.48
4:O:132:LEU:HG	4:O:161:ILE:HD13	1.95	0.48
5:P:37:ALA:HB2	5:P:50:VAL:HG23	1.95	0.48
7:R:38:ILE:HD11	7:R:194:VAL:HG13	1.95	0.48
8:A:174:ALA:O	8:A:178:ALA:N	2.40	0.48
9:B:194:VAL:HG12	9:B:196:ASP:H	1.79	0.48
2:f:50:LYS:N	2:f:207:ASN:O	2.44	0.48
10:H:15:LYS:HD2	10:H:119:PRO:HG2	1.95	0.48
12:U:172:MET:HE1	12:U:213:ARG:HB2	1.95	0.48
15:1:205:ASP:OD1	15:1:206:LEU:N	2.46	0.48
11:I:164:LEU:HB3	11:I:178:PHE:CE2	2.49	0.48
12:J:161:ASP:OD1	12:J:162:SER:N	2.46	0.48
13:K:171:ASP:OD1	13:K:172:MET:N	2.46	0.48
15:X:133:VAL:HG12	15:X:135:ALA:H	1.79	0.48
14:Z:135:MET:O	14:Z:138:MET:HG2	2.14	0.48
6:c:89:ARG:NH1	12:J:105:HIS:HB3	2.29	0.48
10:S:2:SER:OG	10:S:3:ILE:N	2.47	0.48
9:B:47:PRO:HA	9:B:50:ASN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:94:LEU:HD11	8:D:175:VAL:HB	1.96	0.48
13:K:78:LEU:HD13	14:Z:153:TYR:CE2	2.49	0.48
12:U:142:ASP:OD1	12:U:146:LYS:N	2.46	0.48
14:W:135:MET:O	14:W:138:MET:HG2	2.14	0.48
6:Q:182:CYS:HB3	6:Q:186:GLU:HB2	1.96	0.48
9:C:177:TYR:OH	9:C:205:ASP:OD1	2.29	0.48
8:D:229:ASN:ND2	8:D:232:GLY:HA2	2.29	0.48
8:D:231:LYS:C	8:D:233:GLU:N	2.70	0.48
7:d:48:PHE:HZ	7:d:139:GLY:H	1.61	0.48
2:f:143:ARG:HE	2:f:145:TYR:HE1	1.61	0.48
16:Y:110:ASN:HB2	16:Y:113:LEU:HB2	1.96	0.48
10:H:44:PRO:HA	10:H:50:TYR:CD1	2.48	0.48
11:I:41:LYS:HD3	11:I:107:TYR:HD2	1.79	0.48
11:T:44:LEU:HD11	11:T:102:LEU:HD13	1.95	0.48
12:U:59:GLU:HB2	12:U:64:HIS:NE2	2.28	0.48
4:a:80:ALA:HA	4:a:129:ILE:HD13	1.95	0.47
4:a:136:PHE:CD1	4:a:142:PRO:HA	2.49	0.47
5:b:182:GLN:HG2	6:c:56:LEU:HG	1.96	0.47
6:c:62:LYS:NZ	6:c:78:THR:HG22	2.29	0.47
7:d:135:SER:HB2	7:d:154:PRO:HD3	1.95	0.47
10:H:45:MET:HE3	10:H:71:LEU:HD22	1.96	0.47
13:K:118:ASP:HA	13:K:121:LEU:HD12	1.96	0.47
10:S:164:PHE:HE1	10:S:189:ILE:HG13	1.78	0.47
13:V:218:MET:HG2	13:V:221:LEU:HD12	1.95	0.47
5:P:26:TYR:HA	5:P:29:GLU:HB3	1.96	0.47
14:W:37:ASP:OD1	14:W:53:LYS:NZ	2.47	0.47
1:L:47:CYS:SG	1:L:191:PHE:HA	2.54	0.47
5:P:121:LEU:HD21	6:Q:83:LEU:HB2	1.97	0.47
8:A:127:HIS:ND1	9:B:228:ASP:OD2	2.43	0.47
3:g:184:MET:HE2	3:g:192:LEU:HD22	1.96	0.47
5:P:99:HIS:HB2	5:P:107:MET:HE3	1.96	0.47
6:Q:88:MET:HE2	6:Q:112:ILE:HG13	1.97	0.47
1:e:153:LYS:HB3	1:e:163:PHE:CE2	2.49	0.47
10:H:98:LYS:HG3	10:H:103:TYR:CZ	2.49	0.47
14:W:181:LEU:HB2	14:W:216:PHE:CD2	2.50	0.47
15:X:60:THR:HA	15:X:66:ALA:H	1.80	0.47
7:R:22:PHE:CE1	9:C:145:GLY:HA2	2.50	0.47
5:b:202:LEU:HA	5:b:205:VAL:HG22	1.96	0.47
6:c:40:SER:HB3	6:c:187:LEU:HD21	1.96	0.47
1:e:55:LYS:HG2	1:e:57:PRO:HD3	1.95	0.47
16:Y:117:MET:HG2	16:Y:124:CYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:127:TRP:HZ3	16:2:158:MET:HB3	1.79	0.47
1:L:38:THR:HA	1:L:169:GLY:HA3	1.97	0.47
5:P:99:HIS:CE1	5:P:103:TYR:HD2	2.32	0.47
7:R:35:SER:HB3	7:R:66:ARG:HH12	1.80	0.47
4:a:127:PHE:HB3	4:a:129:ILE:HG12	1.96	0.47
3:g:2:SER:OG	3:g:3:ARG:N	2.47	0.47
13:K:94:THR:HB	13:K:130:PRO:HG3	1.96	0.47
10:S:125:ASP:OD1	10:S:126:LEU:N	2.44	0.47
16:2:89:ASP:HB2	16:2:243:GLY:O	2.15	0.47
1:L:29:PHE:CE2	8:A:236:PRO:HG3	2.49	0.47
4:O:49:SER:HB3	4:O:205:ASN:HD21	1.80	0.47
5:P:54:ILE:HG13	5:P:61:PRO:HB3	1.96	0.47
4:a:88:ARG:HD3	11:I:69:MET:HB3	1.97	0.47
5:b:41:GLN:HE22	5:b:164:GLN:HE21	1.62	0.47
5:b:169:ALA:HB3	5:b:178:GLN:HB2	1.97	0.47
12:J:66:ARG:HD3	13:K:196:ARG:HH21	1.80	0.47
13:K:153:ASN:O	13:K:172:MET:HB2	2.13	0.47
13:V:104:ASP:HB3	13:V:151:LEU:HD22	1.97	0.47
16:Y:109:ILE:H	16:Y:114:LEU:HA	1.79	0.47
16:Y:116:THR:OG1	16:Y:172:MET:N	2.47	0.47
16:Y:199:SER:HB3	16:Y:208:TYR:CE1	2.49	0.47
14:Z:28:PHE:HE2	14:Z:33:VAL:HG23	1.80	0.47
10:H:33:GLN:HE21	16:2:238:ARG:HH21	1.62	0.47
13:K:104:ASP:HB3	13:K:151:LEU:HD23	1.97	0.47
12:U:196:LEU:HG	12:U:200:MET:HE2	1.96	0.47
1:L:155:ASP:OD1	1:L:159:TYR:N	2.47	0.47
4:O:94:HIS:HD2	4:O:102:VAL:HA	1.80	0.47
8:F:10:SER:HB3	8:F:13:ALA:HB3	1.97	0.47
4:a:40:ILE:HG21	4:a:184:ASP:HB3	1.97	0.47
6:c:18:ARG:HH21	6:c:23:GLU:HG2	1.80	0.47
2:f:50:LYS:NZ	2:f:62:VAL:O	2.41	0.47
10:H:27:ARG:NH1	10:H:180:VAL:O	2.48	0.47
10:H:32:ALA:O	16:2:240:SER:N	2.46	0.47
13:V:50:MET:CE	13:V:103:ALA:CB	2.93	0.47
1:e:232:GLU:HA	1:e:235:ILE:HD12	1.96	0.47
11:I:18:ASP:HA	11:I:178:PHE:HD1	1.80	0.47
11:T:38:MET:HE3	11:T:44:LEU:HB3	1.96	0.47
13:V:171:ASP:OD1	13:V:172:MET:N	2.47	0.47
15:X:40:THR:HG23	15:X:72:LYS:HE2	1.97	0.47
8:F:7:VAL:HG11	9:G:29:LEU:HD12	1.97	0.46
1:e:116:LYS:HG2	1:e:160:TYR:OH	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:154:TRP:O	15:X:242:ARG:NH2	2.47	0.46
16:2:172:MET:HE3	16:2:200:THR:HG22	1.97	0.46
4:a:195:LEU:O	4:a:199:VAL:HG23	2.15	0.46
13:K:227:ARG:NH1	14:Z:44:GLU:OE2	2.45	0.46
13:V:169:TYR:HB2	13:V:182:LEU:HD13	1.96	0.46
6:Q:10:VAL:HG13	6:Q:19:ILE:HG21	1.98	0.46
8:F:57:LEU:HB3	8:F:196:GLU:HG2	1.97	0.46
12:J:83:SER:O	12:J:135:TYR:N	2.40	0.46
12:U:151:SER:HB2	12:U:164:LYS:HG3	1.97	0.46
13:V:167:LEU:HG	13:V:182:LEU:HD12	1.98	0.46
13:V:211:ARG:NH1	13:V:245:GLU:OE2	2.48	0.46
13:V:221:LEU:O	13:V:225:ASP:HB3	2.14	0.46
15:X:51:VAL:HG13	15:X:147:PRO:HB3	1.98	0.46
15:1:40:THR:HG23	15:1:72:LYS:HE2	1.97	0.46
3:N:135:LEU:HG	3:N:164:ILE:HD13	1.97	0.46
6:Q:15:PRO:HG2	9:G:144:ASP:OD2	2.15	0.46
9:G:239:LYS:H	9:G:240:PRO:HD3	1.80	0.46
4:a:78:ALA:O	3:g:119:GLN:NE2	2.49	0.46
13:K:89:ARG:NH1	13:K:91:ASN:O	2.48	0.46
3:N:8:ARG:HB3	3:N:11:ILE:HG12	1.97	0.46
9:E:211:ASP:OD1	9:E:215:MET:HG3	2.15	0.46
7:d:142:SER:HB3	7:d:145:ASP:HB2	1.96	0.46
12:J:120:LEU:HA	12:J:123:ILE:HD12	1.98	0.46
13:V:137:LEU:HD23	13:V:157:ILE:HD11	1.97	0.46
16:Y:91:ARG:O	16:Y:105:LYS:NZ	2.41	0.46
1:L:65:THR:HG21	7:R:160:GLY:HA3	1.96	0.46
5:P:18:GLU:OE1	5:P:20:ARG:NH2	2.48	0.46
8:A:51:SER:HB3	8:A:103:LEU:HD21	1.98	0.46
8:D:57:LEU:O	8:D:61:ARG:HG2	2.15	0.46
6:c:47:VAL:HG13	6:c:212:ILE:HG22	1.96	0.46
10:S:20:VAL:HG23	10:S:190:ILE:HD13	1.98	0.46
9:G:228:ASP:O	9:G:232:LYS:HG3	2.16	0.46
3:g:86:LEU:HD22	3:g:114:LEU:HD11	1.96	0.46
3:N:155:ASN:ND2	8:D:238:MET:HG2	2.28	0.46
5:P:123:PHE:CE2	5:P:136:PRO:HA	2.51	0.46
8:F:167:TYR:OH	8:F:195:ASP:OD1	2.33	0.46
4:a:18:GLN:HG3	4:a:126:PRO:HG3	1.96	0.46
6:c:123:TYR:CZ	3:g:2:SER:HA	2.51	0.46
10:S:44:PRO:HA	10:S:50:TYR:HD1	1.81	0.46
16:Y:138:TYR:CD2	16:Y:146:ILE:HB	2.51	0.46
8:A:32:LEU:HA	8:A:36:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:211:ASP:OD1	9:E:211:ASP:O	2.33	0.46
6:c:146:GLN:NE2	6:c:161:ILE:HG21	2.30	0.46
10:H:48:ARG:NH2	10:H:192:LYS:O	2.39	0.46
10:S:16:GLY:N	10:S:19:CYS:O	2.45	0.46
11:T:25:ILE:HG13	11:T:26:VAL:HG13	1.97	0.46
16:Y:187:ASP:OD1	16:Y:188:GLU:N	2.46	0.46
14:Z:21:THR:N	14:Z:189:SER:OG	2.47	0.46
1:L:181:LYS:O	1:L:185:LYS:NZ	2.43	0.46
5:P:157:ASP:OD1	5:P:159:SER:OG	2.32	0.46
9:E:139:ILE:HG21	8:F:149:ARG:HH12	1.81	0.46
13:V:189:TYR:HB3	15:X:171:ASP:HB3	1.98	0.46
3:N:155:ASN:ND2	8:D:238:MET:C	2.74	0.45
15:1:182:GLN:O	15:1:185:MET:HG3	2.17	0.45
8:F:174:ALA:HB1	8:F:191:VAL:HB	1.97	0.45
3:g:79:ILE:HG22	3:g:81:SER:H	1.81	0.45
3:g:86:LEU:HD21	3:g:130:PHE:CE2	2.51	0.45
11:I:138:LEU:HD23	16:2:205:SER:O	2.16	0.45
10:S:198:ARG:NH2	15:1:250:VAL:HG22	2.31	0.45
12:U:176:LEU:HD13	12:U:206:VAL:HG12	1.97	0.45
14:Z:56:PRO:HA	14:Z:62:TYR:HD1	1.80	0.45
4:O:41:VAL:HG13	4:O:136:PHE:HE1	1.82	0.45
9:C:43:PHE:CE2	9:C:49:LEU:HD22	2.51	0.45
9:C:191:GLN:HG3	9:G:186:THR:HG23	1.97	0.45
9:G:49:LEU:HD22	9:G:213:ARG:HA	1.98	0.45
7:d:109:LEU:HB2	7:d:140:SER:OG	2.16	0.45
3:g:32:GLY:HA2	3:g:50:ARG:HD3	1.98	0.45
13:K:234:ILE:HD12	13:K:248:LEU:HD12	1.98	0.45
12:U:138:ILE:HB	12:U:150:TYR:HB2	1.98	0.45
12:U:239:ARG:NE	12:U:241:ASP:OD1	2.37	0.45
15:X:165:ALA:HB3	15:X:174:ILE:HG13	1.97	0.45
16:Y:197:MET:HE2	16:Y:211:MET:HE3	1.98	0.45
3:N:1:MET:CE	7:R:128:ALA:HA	2.46	0.45
4:O:31:THR:OG1	4:O:163:ARG:O	2.22	0.45
4:O:109:ARG:HH21	16:2:141:ARG:HE	1.64	0.45
9:E:29:LEU:HD23	9:E:33:PHE:HD2	1.81	0.45
4:a:26:VAL:HA	4:a:75:GLY:HA2	1.98	0.45
3:g:44:LEU:HB3	3:g:215:THR:HG22	1.99	0.45
12:J:49:SER:OG	12:J:226:VAL:HB	2.16	0.45
12:U:65:THR:HA	13:V:196:ARG:NH2	2.31	0.45
15:1:47:PHE:HE2	15:1:52:ILE:HG13	1.80	0.45
3:N:233:VAL:HA	3:N:236:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:180:ALA:C	4:O:181:ILE:HG13	2.41	0.45
6:Q:183:ASN:O	6:Q:187:LEU:HG	2.17	0.45
9:G:61:LEU:O	9:G:198:ARG:NH2	2.49	0.45
4:a:116:GLN:HE22	5:b:84:ASP:HA	1.81	0.45
5:b:129:ASP:HB2	5:b:130:PRO:HD2	1.97	0.45
1:e:38:THR:HG21	1:e:206:LEU:HD11	1.98	0.45
13:V:51:VAL:HG23	13:V:102:TYR:HB3	1.98	0.45
16:2:105:LYS:HB3	16:2:117:MET:HB3	1.99	0.45
4:O:51:ALA:O	4:O:53:LEU:HG	2.16	0.45
5:P:40:ILE:HD11	5:P:198:SER:HB2	1.99	0.45
5:P:191:LEU:HD13	5:P:221:GLN:HE21	1.81	0.45
8:F:114:LEU:HD11	8:F:212:PHE:HB2	1.97	0.45
5:b:146:VAL:HG22	5:b:151:PRO:HB3	1.97	0.45
11:I:183:ILE:HG12	11:I:188:ILE:HG12	1.99	0.45
12:J:85:PHE:CZ	13:K:173:LEU:HB3	2.49	0.45
11:T:29:LYS:HD2	16:2:194:SER:O	2.17	0.45
13:V:59:LEU:HD11	13:V:199:LEU:HD21	1.97	0.45
2:M:39:LYS:HG3	2:M:44:VAL:HG22	1.99	0.45
2:M:118:MET:HG2	2:M:130:PHE:HD2	1.82	0.45
2:M:157:ALA:HB3	3:N:58:GLU:H	1.80	0.45
4:O:184:ASP:OD2	4:O:212:ARG:NH1	2.50	0.45
6:Q:44:ALA:HB2	6:Q:142:PRO:HB2	1.98	0.45
9:E:54:LEU:HB3	9:E:206:GLU:HG2	1.99	0.45
3:g:53:HIS:HB3	3:g:56:LEU:HG	1.98	0.45
3:g:77:ALA:HB3	3:g:164:ILE:HD12	1.99	0.45
14:W:146:ILE:HB	14:W:151:SER:HB2	1.99	0.45
1:L:53:GLN:NE2	1:L:214:GLU:O	2.50	0.45
2:M:118:MET:HG2	2:M:130:PHE:CD2	2.52	0.45
7:d:216:TRP:HB3	7:d:221:THR:HG21	1.97	0.45
13:V:61:PHE:CE2	13:V:66:VAL:HG23	2.52	0.45
15:X:47:PHE:CZ	15:X:187:LEU:HD13	2.52	0.45
2:M:53:LYS:HB2	2:M:57:TYR:HE2	1.82	0.45
10:H:190:ILE:HA	10:H:195:ILE:HG12	1.97	0.45
8:A:172:GLY:HA2	9:B:194:VAL:HG11	1.98	0.45
4:a:5:ARG:NH1	3:g:2:SER:O	2.45	0.45
5:b:60:GLU:HG2	5:b:62:SER:H	1.82	0.45
7:d:64:ASN:OD1	7:d:82:LEU:HD13	2.16	0.45
1:e:70:PHE:CD2	1:e:91:VAL:HG21	2.52	0.45
12:J:55:THR:OG1	12:J:220:ALA:HB3	2.17	0.45
14:W:54:LEU:HD13	14:W:196:ALA:HB2	1.98	0.45
2:M:93:LEU:HD21	2:M:113:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:100:VAL:HA	10:H:93:ASN:ND2	2.31	0.44
14:Z:27:GLU:HA	14:Z:32:VAL:HG12	1.98	0.44
1:L:206:LEU:HD22	1:L:210:PHE:HZ	1.82	0.44
9:B:172:THR:HG22	9:B:176:LYS:HE3	1.99	0.44
9:C:121:ILE:HG12	9:C:219:ILE:HD11	1.99	0.44
6:c:109:VAL:HA	6:c:112:ILE:HD12	1.97	0.44
3:g:49:ARG:HH12	3:g:58:GLU:HG2	1.82	0.44
11:I:35:MET:HG2	11:I:45:LEU:HD11	1.98	0.44
13:K:160:TYR:HA	13:K:165:SER:HA	1.99	0.44
9:G:239:LYS:H	9:G:240:PRO:CD	2.31	0.44
1:L:62:ASP:OD1	1:L:63:SER:N	2.50	0.44
4:O:98:VAL:HG12	4:O:100:ASP:H	1.82	0.44
8:D:52:LEU:HB3	8:D:203:ARG:HD3	1.99	0.44
10:S:16:GLY:HA3	10:S:163:LEU:HD11	1.98	0.44
12:U:120:LEU:HA	12:U:123:ILE:HD12	1.98	0.44
1:e:206:LEU:HD12	1:e:210:PHE:HZ	1.83	0.44
10:S:44:PRO:HA	10:S:50:TYR:CD1	2.52	0.44
10:S:164:PHE:CE1	10:S:189:ILE:HG13	2.52	0.44
14:W:58:HIS:HB3	14:W:61:ILE:HB	1.99	0.44
16:2:73:THR:HG23	16:2:105:LYS:HE2	1.99	0.44
9:C:156:VAL:HG12	9:C:160:MET:HE2	2.00	0.44
8:F:32:LEU:HA	8:F:36:LEU:HD12	2.00	0.44
9:G:27:ASN:O	9:G:31:SER:HB3	2.18	0.44
7:d:50:VAL:HB	7:d:213:GLU:HB2	2.00	0.44
11:I:28:MET:HE1	16:Y:185:TYR:CZ	2.53	0.44
3:N:43:VAL:HG21	3:N:137:ILE:HB	1.99	0.44
9:C:172:THR:HG22	9:C:176:LYS:HE3	1.99	0.44
12:J:40:VAL:HG23	12:J:83:SER:HB2	1.99	0.44
10:S:159:ASP:OD1	10:S:162:HIS:ND1	2.31	0.44
11:T:29:LYS:HD3	11:T:32:HIS:HB2	1.98	0.44
13:V:105:PHE:CE2	13:V:109:LYS:HD2	2.52	0.44
13:V:223:TYR:HB3	14:W:49:ARG:HD3	2.00	0.44
15:X:136:SER:OG	15:X:166:LEU:HD13	2.18	0.44
1:L:90:GLN:HE21	1:L:134:LEU:HD12	1.82	0.44
10:H:195:ILE:HD12	15:X:258:LEU:HD21	2.00	0.44
12:U:56:ARG:NH1	12:U:215:VAL:O	2.51	0.44
15:X:98:ALA:O	15:X:102:MET:HG2	2.18	0.44
3:N:69:ASN:OD1	3:N:72:MET:N	2.51	0.44
4:O:13:ASP:HB2	4:O:15:HIS:CE1	2.53	0.44
4:O:146:GLN:OE1	4:O:159:ASN:ND2	2.31	0.44
5:P:181:LEU:HD22	5:P:185:TYR:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:117:LEU:HD13	9:B:216:VAL:HG22	1.98	0.44
8:D:47:LEU:HD12	8:D:210:ARG:HH11	1.83	0.44
11:T:101:ASN:HB3	11:T:132:HIS:ND1	2.33	0.44
12:U:215:VAL:O	15:X:206:LEU:HD22	2.18	0.44
13:V:82:ARG:NH2	14:W:219:GLU:O	2.51	0.44
16:2:138:TYR:CD2	16:2:146:ILE:HB	2.52	0.44
9:E:4:LEU:HD22	8:F:33:TYR:HB2	1.99	0.43
9:E:117:LEU:HD13	9:E:216:VAL:HG22	1.99	0.43
8:F:25:PHE:CE1	8:F:128:LEU:HD21	2.53	0.43
4:a:65:LEU:HD22	4:a:87:ALA:HB3	1.99	0.43
5:b:81:LEU:HD12	5:b:138:GLY:HA3	1.99	0.43
7:d:69:ASN:ND2	13:K:120:GLU:O	2.51	0.43
1:e:210:PHE:CD2	1:e:215:ILE:HD13	2.53	0.43
14:W:210:GLY:HA2	14:W:213:LEU:HG	2.00	0.43
8:A:52:LEU:HD23	8:A:103:LEU:HD13	2.00	0.43
6:c:120:THR:HB	7:d:130:ARG:HH21	1.83	0.43
6:c:193:ARG:HG2	6:c:196:ARG:HE	1.83	0.43
12:J:64:HIS:HB3	13:K:177:TYR:OH	2.18	0.43
15:1:67:ASP:HB3	15:1:70:CYS:HB2	2.00	0.43
16:2:197:MET:HE2	16:2:211:MET:HE3	2.00	0.43
3:N:45:LEU:HD21	3:N:75:SER:HB2	1.99	0.43
4:O:137:ASP:OD1	4:O:138:PHE:N	2.47	0.43
8:A:224:LEU:HD21	9:C:4:LEU:HB2	2.00	0.43
6:c:76:GLY:HA3	6:c:130:VAL:HA	2.00	0.43
7:d:8:TYR:HE1	1:e:11:ARG:HB3	1.83	0.43
2:f:118:MET:HA	2:f:130:PHE:HE2	1.83	0.43
14:Z:62:TYR:CD2	14:Z:198:ILE:HD11	2.53	0.43
5:b:70:ILE:HG23	5:b:93:ARG:HG2	2.01	0.43
7:d:127:SER:OG	2:f:6:TYR:OH	2.25	0.43
12:J:127:ARG:HG3	12:J:132:TYR:CZ	2.54	0.43
11:T:7:ILE:O	11:T:14:LEU:N	2.42	0.43
13:V:86:ARG:NH2	13:V:99:SER:HA	2.33	0.43
14:W:22:THR:H	14:W:37:ASP:CG	2.26	0.43
16:Y:109:ILE:HD13	16:Y:131:LEU:HD23	2.01	0.43
4:O:188:ILE:HG23	4:O:208:LEU:HD13	2.00	0.43
8:F:113:THR:O	8:F:117:LYS:HG2	2.19	0.43
16:2:80:PHE:CE1	16:2:82:HIS:HB2	2.53	0.43
8:A:112:TRP:HB3	9:B:210:ARG:HH21	1.84	0.43
9:B:33:PHE:HB2	9:B:34:PRO:HD3	2.01	0.43
8:F:171:ARG:HB3	9:G:196:ASP:OD2	2.19	0.43
5:b:166:ASP:HB3	5:b:185:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:54:VAL:HG13	7:d:59:TYR:HD2	1.84	0.43
10:S:200:LEU:HD22	15:1:248:THR:HG21	2.01	0.43
11:T:42:ILE:HG12	11:T:106:GLY:HA3	2.00	0.43
13:V:98:ALA:HA	13:V:155:MET:HA	2.00	0.43
13:V:105:PHE:O	13:V:109:LYS:N	2.41	0.43
8:D:101:LEU:HD11	8:D:171:ARG:HH22	1.84	0.43
6:c:173:GLU:HG3	7:d:57:LYS:HD2	2.00	0.43
3:g:136:TYR:HB2	3:g:148:TYR:HB2	2.00	0.43
12:U:192:VAL:HB	12:U:198:ARG:HH12	1.83	0.43
12:U:85:PHE:CZ	13:V:173:LEU:HB3	2.53	0.43
6:Q:6:TYR:OH	7:R:9:ASP:OD2	2.25	0.43
7:R:67:LEU:HD13	7:R:215:SER:HB2	2.01	0.43
9:C:236:LYS:HZ2	9:G:143:GLU:C	2.27	0.43
8:D:237:SER:C	8:D:239:TYR:N	2.76	0.43
9:G:114:LEU:O	9:G:118:LYS:HG3	2.19	0.43
5:b:8:TYR:OH	3:g:11:ILE:HG21	2.19	0.43
10:H:95:LEU:HD11	10:H:107:PRO:HG2	2.01	0.43
14:Z:152:THR:HA	14:Z:155:TYR:HE2	1.84	0.43
15:1:98:ALA:O	15:1:102:MET:HG2	2.19	0.43
16:2:79:LYS:HA	16:2:84:VAL:HG22	2.00	0.43
2:M:97:TYR:CE2	2:M:105:ILE:HA	2.54	0.43
8:F:221:SER:HA	8:F:224:LEU:HG	2.01	0.43
4:a:16:LEU:HD13	4:a:19:VAL:HG21	2.01	0.43
7:d:88:LEU:HD21	7:d:132:PHE:CE2	2.54	0.43
12:J:138:ILE:O	12:J:149:VAL:HA	2.19	0.43
16:2:84:VAL:HB	16:2:251:MET:HG3	2.00	0.43
3:N:1:MET:CE	7:R:128:ALA:CB	2.97	0.42
4:O:45:VAL:HG11	4:O:61:LYS:HB2	2.01	0.42
4:O:76:LEU:CA	8:D:239:TYR:HB2	2.47	0.42
7:d:17:PRO:HA	1:e:27:TYR:CD1	2.54	0.42
10:S:15:LYS:HB2	10:S:121:ILE:HD13	2.00	0.42
10:S:177:ARG:HA	16:Y:98:ILE:HD12	2.01	0.42
12:U:117:ALA:HA	12:U:152:PHE:HZ	1.84	0.42
12:U:159:GLN:OE1	16:2:103:VAL:HG22	2.19	0.42
14:W:183:MET:HB3	14:W:190:GLY:HA2	2.00	0.42
9:E:37:ILE:HG12	9:E:223:TYR:HB3	2.01	0.42
7:d:80:GLY:HA3	7:d:134:CYS:HA	2.02	0.42
11:T:145:ARG:NH2	16:Y:210:VAL:HB	2.34	0.42
5:P:70:ILE:HA	5:P:93:ARG:HG2	2.01	0.42
8:A:183:HIS:O	9:C:104:VAL:N	2.50	0.42
9:C:46:GLU:HG2	9:C:48:ALA:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:159:LEU:HD13	9:E:229:ILE:HD13	2.01	0.42
9:E:230:ILE:O	9:E:234:PHE:HB2	2.19	0.42
6:c:95:SER:HB2	6:c:103:LEU:HB2	2.02	0.42
7:d:45:GLY:HA3	7:d:218:GLY:HA3	2.01	0.42
10:H:28:PHE:O	10:H:35:VAL:N	2.48	0.42
14:W:24:MET:HB3	14:W:179:ILE:HD11	2.01	0.42
15:1:43:ALA:O	15:1:54:GLY:N	2.48	0.42
3:N:37:ILE:HD12	3:N:44:LEU:HD23	2.00	0.42
3:N:148:TYR:HD1	3:N:158:GLY:HA2	1.85	0.42
6:Q:15:PRO:HA	7:R:26:TYR:CD1	2.54	0.42
2:f:77:SER:HB3	2:f:163:MET:HG2	2.01	0.42
3:g:8:ARG:HB3	3:g:11:ILE:CG1	2.50	0.42
10:H:149:MET:HE3	10:H:153:LEU:HD11	2.01	0.42
13:K:62:GLU:N	13:K:205:LEU:O	2.44	0.42
13:V:62:GLU:N	13:V:205:LEU:O	2.47	0.42
5:P:41:GLN:NE2	5:P:151:PRO:O	2.53	0.42
7:R:22:PHE:CZ	9:C:145:GLY:HA2	2.55	0.42
8:F:185:MET:HA	8:F:188:ARG:NE	2.34	0.42
12:J:92:LEU:HD11	12:J:120:LEU:HD11	2.01	0.42
13:K:84:ILE:HG22	14:W:140:ILE:HD12	2.02	0.42
12:U:173:LEU:HD21	12:U:210:ALA:HB2	2.00	0.42
16:2:268:MET:O	16:2:272:ARG:N	2.42	0.42
1:L:28:ALA:O	1:L:32:ILE:HD12	2.19	0.42
1:L:88:ARG:NE	7:R:114:ASP:OD1	2.49	0.42
5:P:81:LEU:HD23	5:P:84:ASP:OD2	2.20	0.42
9:C:61:LEU:HG	9:C:63:ILE:H	1.84	0.42
1:e:93:ARG:HA	1:e:96:TYR:CD2	2.55	0.42
2:f:185:GLU:HG2	2:f:234:ALA:HB1	2.01	0.42
10:H:95:LEU:HD23	10:H:103:TYR:HD2	1.85	0.42
15:X:233:LYS:O	15:X:235:ILE:N	2.53	0.42
16:Y:245:VAL:HG12	16:Y:263:ASP:HA	2.01	0.42
14:Z:96:VAL:HG11	14:Z:130:GLN:HB2	2.01	0.42
16:2:110:ASN:HD21	16:2:135:CYS:HB3	1.84	0.42
4:O:32:ALA:HB3	4:O:161:ILE:HG13	2.02	0.42
5:P:46:VAL:HG11	5:P:144:GLY:HA3	2.01	0.42
7:R:214:LEU:HB2	7:R:228:VAL:HG11	2.02	0.42
8:F:64:LEU:H	8:F:192:HIS:CE1	2.38	0.42
1:e:49:VAL:HG22	1:e:219:VAL:HG12	2.01	0.42
10:H:83:LYS:HG2	10:H:114:PRO:HD2	2.02	0.42
10:S:72:ASN:O	10:S:76:LEU:N	2.51	0.42
10:S:84:PRO:HD3	10:S:114:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:192:ASP:OD1	11:T:193:ASN:N	2.52	0.42
13:V:131:LYS:O	13:V:135:SER:N	2.46	0.42
15:X:60:THR:CG2	15:X:65:VAL:HG22	2.49	0.42
15:X:76:ILE:HD11	15:X:95:THR:HB	2.02	0.42
16:2:80:PHE:HE1	16:2:82:HIS:HB2	1.84	0.42
3:N:143:TYR:HB3	3:N:146:GLN:NE2	2.35	0.42
3:N:160:LYS:HB3	3:N:179:TYR:OH	2.20	0.42
7:R:80:GLY:HA3	7:R:134:CYS:HA	2.02	0.42
8:A:168:PHE:CE2	9:B:203:GLU:HG3	2.55	0.42
8:A:175:VAL:O	8:A:179:SER:N	2.52	0.42
9:B:22:CYS:SG	9:B:134:TRP:NE1	2.74	0.42
9:B:57:LEU:HD22	9:B:209:TYR:CD1	2.54	0.42
8:D:36:LEU:HB2	8:D:37:PRO:HD3	2.02	0.42
5:b:21:LEU:HB2	5:b:24:VAL:HB	2.02	0.42
6:c:19:ILE:HG22	6:c:22:ILE:H	1.84	0.42
7:d:70:VAL:HG13	7:d:92:ALA:HB1	2.01	0.42
7:d:99:PHE:CE1	7:d:103:PHE:HD2	2.38	0.42
1:e:103:TYR:HA	15:X:120:ARG:HH21	1.85	0.42
10:H:130:PRO:HD2	15:X:92:GLU:HG3	2.02	0.42
11:I:87:ASN:O	11:I:91:TYR:CE2	2.73	0.42
12:J:159:GLN:HG3	16:Y:103:VAL:HA	2.01	0.42
12:J:239:ARG:CB	15:I:234:PRO:HG2	2.49	0.42
10:S:113:ASP:CB	10:S:118:LYS:HB3	2.50	0.42
13:V:78:LEU:HD13	14:W:153:TYR:CZ	2.54	0.42
6:Q:19:ILE:HG22	6:Q:22:ILE:H	1.85	0.42
7:R:203:ASP:OD1	7:R:204:GLU:N	2.49	0.42
8:F:49:GLU:HG2	8:F:51:SER:H	1.85	0.42
5:b:85:ALA:O	5:b:89:ILE:HG13	2.20	0.42
12:J:63:ILE:O	13:K:192:GLN:NE2	2.37	0.42
13:K:106:GLN:HA	13:K:109:LYS:HB3	2.02	0.42
12:U:55:THR:CG2	12:U:222:LYS:HE3	2.48	0.42
16:Y:134:GLU:HA	16:Y:137:LEU:HB2	2.02	0.42
16:2:233:VAL:HG21	16:2:271:TYR:HE2	1.84	0.42
1:L:237:ALA:O	1:L:241:ALA:HB3	2.19	0.42
3:N:1:MET:HE1	7:R:128:ALA:CA	2.50	0.42
4:O:23:GLN:OE1	9:E:246:GLY:HA2	2.20	0.42
4:a:199:VAL:HG12	4:a:201:SER:H	1.83	0.42
10:H:4:MET:SD	10:H:126:LEU:HD21	2.60	0.42
12:J:73:LYS:HG2	12:J:79:VAL:HG22	2.02	0.42
13:K:82:ARG:NH1	14:Z:218:ASP:HA	2.35	0.42
10:S:14:MET:HE3	10:S:154:TRP:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:15:PRO:HA	7:R:26:TYR:CE1	2.55	0.41
6:Q:109:VAL:HG21	6:Q:145:PHE:HD2	1.84	0.41
8:F:168:PHE:CE2	9:G:203:GLU:HG3	2.55	0.41
9:G:240:PRO:HB2	9:G:241:ARG:H	1.61	0.41
5:b:66:LYS:HG2	5:b:78:MET:HE2	2.02	0.41
6:c:40:SER:HB3	6:c:187:LEU:HD11	2.01	0.41
6:c:121:GLN:HA	7:d:130:ARG:HG2	2.02	0.41
10:H:59:ASP:HA	10:H:62:THR:HB	2.00	0.41
11:I:25:ILE:HG13	11:I:26:VAL:HG13	2.01	0.41
11:T:138:LEU:HD23	16:Y:205:SER:O	2.19	0.41
16:2:127:TRP:CZ3	16:2:158:MET:HB3	2.55	0.41
3:N:68:LEU:H	3:N:73:ALA:HA	1.85	0.41
4:O:64:ALA:HA	4:O:70:CYS:HA	2.02	0.41
5:P:97:GLN:HB3	16:2:133:LYS:HG3	2.02	0.41
7:d:78:VAL:HG12	7:d:136:PHE:HB3	2.01	0.41
11:I:64:VAL:HG13	11:I:75:LEU:HD12	2.02	0.41
10:S:116:THR:HB	10:S:117:PHE:H	1.50	0.41
4:O:166:LYS:HG3	4:O:169:ARG:HH21	1.85	0.41
8:A:93:PHE:HD1	9:B:65:VAL:HG21	1.85	0.41
9:C:118:LYS:HE2	9:C:174:ILE:HG21	2.02	0.41
5:b:16:SER:OG	5:b:20:ARG:N	2.49	0.41
1:e:119:ALA:O	1:e:122:SER:OG	2.37	0.41
10:H:194:LYS:HG2	15:X:257:PRO:HA	2.02	0.41
11:I:9:GLY:HA3	11:I:12:TYR:CZ	2.55	0.41
12:J:59:GLU:H	12:J:64:HIS:CD2	2.38	0.41
10:S:201:LYS:HB3	15:1:249:PRO:HG2	2.03	0.41
14:Z:93:PRO:HA	14:Z:94:PRO:HD3	1.98	0.41
1:L:27:TYR:CD1	7:R:17:PRO:HA	2.56	0.41
1:L:32:ILE:HG13	1:L:135:GLY:O	2.19	0.41
4:O:148:ASP:OD2	4:O:150:SER:OG	2.35	0.41
8:F:64:LEU:HD22	8:F:94:LEU:HB3	2.02	0.41
4:a:155:ALA:HB3	5:b:63:SER:HB3	2.02	0.41
5:b:52:LYS:NZ	5:b:61:PRO:HB2	2.36	0.41
7:d:70:VAL:HG23	7:d:76:MET:HB2	2.01	0.41
3:g:175:LEU:O	3:g:179:TYR:HB3	2.21	0.41
10:H:201:LYS:HB2	15:X:251:LEU:HB2	2.01	0.41
11:I:26:VAL:HG21	16:Y:208:TYR:CE2	2.55	0.41
13:K:86:ARG:HH21	13:K:99:SER:HA	1.86	0.41
12:U:97:GLU:HA	12:U:100:LEU:HD12	2.02	0.41
13:V:98:ALA:HB2	13:V:155:MET:HG2	2.03	0.41
15:X:205:ASP:OD1	15:X:206:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:26:TYR:O	5:P:30:ALA:N	2.54	0.41
9:B:140:PRO:HD3	9:B:240:PRO:HG3	2.03	0.41
4:a:125:ARG:HE	3:g:123:GLN:HA	1.85	0.41
5:b:38:ILE:HD11	5:b:177:ALA:HB1	2.02	0.41
11:I:19:ARG:HD3	11:I:177:THR:HG22	2.01	0.41
12:U:213:ARG:NH1	15:X:68:LYS:HG3	2.36	0.41
15:1:77:ALA:HB3	15:1:80:ILE:HB	2.02	0.41
2:M:45:VAL:HG21	2:M:188:ILE:HG12	2.01	0.41
5:P:85:ALA:O	5:P:89:ILE:HG12	2.21	0.41
9:B:214:LEU:O	9:B:218:GLU:HG2	2.21	0.41
8:D:122:ILE:O	8:D:126:GLN:HG2	2.20	0.41
8:F:33:TYR:HD2	8:F:34:ARG:HG3	1.85	0.41
9:G:54:LEU:HD21	9:G:209:TYR:CE2	2.56	0.41
4:a:167:SER:O	4:a:171:PHE:N	2.48	0.41
6:c:132:LEU:O	6:c:146:GLN:HG3	2.19	0.41
6:c:176:MET:HA	6:c:179:PHE:CD2	2.55	0.41
7:d:13:SER:O	1:e:24:GLN:NE2	2.54	0.41
11:I:4:LEU:HB2	11:I:132:HIS:CD2	2.51	0.41
12:J:151:SER:HB2	12:J:164:LYS:HG3	2.03	0.41
12:J:157:SER:HA	16:Y:125:LEU:HD12	2.02	0.41
13:K:223:TYR:OH	13:K:252:THR:HA	2.20	0.41
10:S:27:ARG:HB2	10:S:182:GLY:O	2.21	0.41
10:S:53:LEU:HB2	10:S:60:VAL:HG13	2.01	0.41
11:T:19:ARG:NH2	11:T:31:ASP:HB2	2.35	0.41
13:V:181:SER:HB3	13:V:199:LEU:HD11	2.01	0.41
14:W:42:ALA:N	14:W:45:ALA:O	2.54	0.41
15:X:117:THR:HG22	15:X:121:MET:HE3	2.03	0.41
15:1:60:THR:HA	15:1:66:ALA:H	1.85	0.41
4:O:94:HIS:CD2	4:O:102:VAL:HA	2.55	0.41
5:b:68:VAL:HG23	5:b:76:CYS:HB3	2.03	0.41
5:b:153:LEU:HB3	5:b:165:CYS:O	2.21	0.41
1:e:50:ILE:HG21	1:e:79:VAL:HG11	2.02	0.41
10:H:44:PRO:HA	10:H:50:TYR:HD1	1.85	0.41
13:V:92:ASN:O	13:V:242:VAL:HG23	2.20	0.41
16:2:187:ASP:OD1	16:2:188:GLU:N	2.46	0.41
16:2:200:THR:C	16:2:204:ASN:HB3	2.46	0.41
4:a:61:LYS:HE2	4:a:77:THR:HG22	2.02	0.41
5:b:10:ARG:HD3	5:b:22:PHE:CD2	2.56	0.41
5:b:99:HIS:CD2	5:b:107:MET:HB2	2.56	0.41
6:c:65:HIS:O	6:c:89:ARG:NE	2.50	0.41
10:H:169:GLN:HG3	15:X:243:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:V:73:GLY:N	13:V:81:PHE:O	2.46	0.41
14:W:24:MET:HA	14:W:146:ILE:HG22	2.03	0.41
14:W:170:GLU:O	14:W:174:PHE:N	2.48	0.41
3:N:39:ALA:HB1	3:N:185:THR:HA	2.03	0.41
4:O:25:ALA:HB1	4:O:76:LEU:CD1	2.50	0.41
7:R:109:LEU:HD11	7:R:138:LEU:HB3	2.03	0.41
8:D:176:ALA:O	8:D:179:SER:OG	2.34	0.41
8:D:209:LEU:HG	8:D:213:TYR:HE2	1.85	0.41
8:F:51:SER:HB3	8:F:103:LEU:HD21	2.03	0.41
9:G:33:PHE:CZ	9:G:127:GLN:HB3	2.56	0.41
9:G:199:GLN:HE21	9:G:203:GLU:HG2	1.86	0.41
4:a:66:ASP:OD1	4:a:67:ASP:N	2.49	0.41
4:a:148:ASP:OD1	4:a:149:PRO:HD2	2.21	0.41
5:b:145:GLY:O	5:b:151:PRO:HA	2.20	0.41
6:c:62:LYS:HZ2	6:c:78:THR:HG22	1.84	0.41
7:d:102:ASN:O	14:W:105:ASN:ND2	2.54	0.41
2:f:105:ILE:HD13	2:f:110:LEU:HD13	2.03	0.41
2:f:195:LEU:HD13	2:f:208:ILE:HD12	2.03	0.41
3:g:118:LYS:HG2	3:g:130:PHE:CD2	2.55	0.41
10:H:26:ARG:HB2	10:H:183:MET:O	2.20	0.41
11:I:4:LEU:HD21	11:I:34:LYS:HD3	2.02	0.41
12:J:59:GLU:HB3	12:J:64:HIS:NE2	2.36	0.41
12:J:213:ARG:HG3	10:S:147:TYR:HB3	2.02	0.41
13:K:69:ALA:HB1	13:K:86:ARG:HD3	2.03	0.41
11:T:140:LEU:HD23	11:T:143:LEU:HD12	2.03	0.41
12:U:90:LEU:O	12:U:94:LYS:HG2	2.21	0.41
13:V:52:THR:N	13:V:74:SER:O	2.54	0.41
13:V:181:SER:HB2	13:V:195:LEU:HD13	2.02	0.41
14:W:65:LEU:HG	14:W:72:ALA:HB1	2.03	0.41
8:A:30:GLU:O	8:A:34:ARG:HB2	2.20	0.41
8:A:128:LEU:HD13	8:A:228:VAL:HA	2.03	0.41
8:A:177:LYS:HA	8:A:180:LYS:HG2	2.02	0.41
9:C:27:ASN:O	9:C:31:SER:HB3	2.21	0.41
8:F:57:LEU:HA	8:F:60:LEU:HD12	2.02	0.41
9:G:118:LYS:HB2	9:G:119:PRO:HD3	2.03	0.41
1:e:72:ILE:HG12	1:e:78:CYS:HB2	2.03	0.41
10:S:12:MET:HG3	10:S:138:VAL:HG12	2.02	0.41
10:S:159:ASP:CG	10:S:162:HIS:HD1	2.25	0.41
11:T:11:ASP:C	11:T:113:PRO:HG3	2.46	0.41
14:W:72:ALA:HB1	14:W:118:LEU:HD21	2.03	0.41
14:Z:38:SER:HB3	14:Z:194:TYR:HE2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:139:TRP:CZ2	2:M:142:GLY:HA2	2.57	0.40
4:O:148:ASP:OD1	4:O:149:PRO:HD2	2.21	0.40
6:Q:67:ASP:OD1	6:Q:68:ASN:N	2.51	0.40
9:G:28:LEU:HA	9:G:32:TYR:HB3	2.02	0.40
9:G:152:VAL:HG22	9:G:155:LYS:HD2	2.04	0.40
4:a:98:VAL:HG12	4:a:100:ASP:H	1.87	0.40
2:f:60:ARG:HA	2:f:63:HIS:CE1	2.55	0.40
3:g:197:LEU:O	3:g:201:MET:N	2.33	0.40
10:H:179:ALA:HB1	16:2:240:SER:O	2.21	0.40
11:I:171:PHE:HE2	11:I:173:LEU:HB2	1.84	0.40
11:I:172:ILE:CG2	11:T:173:LEU:HD22	2.50	0.40
13:K:258:HIS:NE2	14:Z:209:LEU:HD21	2.36	0.40
10:S:142:CYS:HB3	10:S:178:ASP:OD2	2.21	0.40
13:V:51:VAL:HG21	13:V:102:TYR:HB3	2.04	0.40
1:L:18:PRO:HG3	9:B:148:PHE:HE2	1.86	0.40
8:A:96:GLY:HA2	8:A:171:ARG:HE	1.86	0.40
8:D:60:LEU:HB3	8:D:199:TYR:CD2	2.57	0.40
9:G:211:ASP:O	9:G:215:MET:HG3	2.21	0.40
4:a:88:ARG:NH1	11:I:69:MET:O	2.54	0.40
1:e:105:TYR:HA	15:X:117:THR:HG23	2.02	0.40
2:f:140:ASN:HB2	2:f:145:TYR:HE2	1.85	0.40
10:H:63:VAL:O	10:H:67:LEU:HG	2.21	0.40
13:K:57:LEU:HD11	13:K:221:LEU:HD11	2.03	0.40
10:S:49:LEU:HD13	10:S:84:PRO:HB3	2.04	0.40
10:S:96:TYR:CD2	10:S:96:TYR:O	2.74	0.40
13:V:192:GLN:HE21	13:V:196:ARG:CZ	2.34	0.40
4:O:47:LYS:NZ	4:O:207:GLU:HB3	2.35	0.40
8:A:114:LEU:HD13	8:A:213:TYR:HE1	1.85	0.40
9:C:106:CYS:SG	9:C:111:VAL:HG21	2.60	0.40
9:C:152:VAL:O	9:C:156:VAL:HG23	2.21	0.40
8:D:60:LEU:HB3	8:D:199:TYR:CE2	2.55	0.40
9:G:236:LYS:HB3	9:G:236:LYS:HE3	1.90	0.40
7:d:36:THR:HG21	7:d:201:VAL:HG11	2.03	0.40
10:S:15:LYS:HA	10:S:20:VAL:HA	2.02	0.40
13:V:54:THR:HG22	13:V:86:ARG:HH12	1.85	0.40
15:X:47:PHE:HE1	15:X:49:ASP:HB2	1.85	0.40
1:L:21:ARG:NH2	1:L:26:GLU:OE1	2.54	0.40
3:N:1:MET:CE	7:R:128:ALA:CA	2.99	0.40
6:Q:39:LYS:HB3	6:Q:144:ILE:HG12	2.02	0.40
9:C:33:PHE:HB2	9:C:34:PRO:HD3	2.04	0.40
1:e:78:CYS:SG	1:e:79:VAL:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:123:TRP:HB3	14:Z:198:ILE:HG22	2.04	0.40
14:Z:162:TYR:HB2	14:Z:174:PHE:CZ	2.56	0.40
14:Z:186:ASP:HB3	14:Z:189:SER:HB2	2.03	0.40
1:L:45:LYS:H	1:L:189:TRP:HB3	1.87	0.40
8:A:12:GLU:OE2	8:A:16:GLN:NE2	2.48	0.40
8:F:52:LEU:HD13	8:F:206:VAL:HG11	2.04	0.40
8:F:132:ILE:HG21	9:G:152:VAL:HG21	2.03	0.40
9:G:41:ASP:OD1	9:G:220:ARG:NH1	2.54	0.40
4:a:50:VAL:HG12	4:a:52:LYS:H	1.86	0.40
5:b:231:LYS:HA	5:b:234:LEU:HB2	2.02	0.40
6:c:152:ASN:OD1	6:c:153:TYR:N	2.54	0.40
15:1:133:VAL:HG12	15:1:135:ALA:H	1.86	0.40
15:1:232:THR:HG23	15:1:234:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	234/246 (95%)	220 (94%)	14 (6%)	0	100	100
1	e	236/246 (96%)	217 (92%)	19 (8%)	0	100	100
2	M	224/234 (96%)	217 (97%)	7 (3%)	0	100	100
2	f	228/234 (97%)	220 (96%)	8 (4%)	0	100	100
3	N	244/261 (94%)	234 (96%)	10 (4%)	0	100	100
3	g	244/261 (94%)	226 (93%)	17 (7%)	1 (0%)	30	67
4	O	230/248 (93%)	220 (96%)	10 (4%)	0	100	100
4	a	230/248 (93%)	218 (95%)	12 (5%)	0	100	100
5	P	232/241 (96%)	218 (94%)	14 (6%)	0	100	100
5	b	232/241 (96%)	224 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Q	233/263 (89%)	217 (93%)	16 (7%)	0	100	100
6	c	233/263 (89%)	224 (96%)	9 (4%)	0	100	100
7	R	238/255 (93%)	230 (97%)	8 (3%)	0	100	100
7	d	238/255 (93%)	227 (95%)	11 (5%)	0	100	100
8	A	205/239 (86%)	204 (100%)	1 (0%)	0	100	100
8	D	203/239 (85%)	193 (95%)	9 (4%)	1 (0%)	25	62
8	F	206/239 (86%)	202 (98%)	4 (2%)	0	100	100
9	B	209/249 (84%)	202 (97%)	6 (3%)	1 (0%)	25	62
9	C	202/249 (81%)	198 (98%)	4 (2%)	0	100	100
9	E	204/249 (82%)	194 (95%)	9 (4%)	1 (0%)	25	62
9	G	201/249 (81%)	194 (96%)	4 (2%)	3 (2%)	8	40
10	H	202/205 (98%)	188 (93%)	14 (7%)	0	100	100
10	S	202/205 (98%)	185 (92%)	16 (8%)	1 (0%)	25	62
11	I	196/201 (98%)	186 (95%)	10 (5%)	0	100	100
11	T	195/201 (97%)	183 (94%)	12 (6%)	0	100	100
12	J	211/241 (88%)	198 (94%)	13 (6%)	0	100	100
12	U	211/241 (88%)	197 (93%)	14 (7%)	0	100	100
13	K	214/264 (81%)	206 (96%)	7 (3%)	1 (0%)	25	62
13	V	214/264 (81%)	203 (95%)	11 (5%)	0	100	100
14	W	197/219 (90%)	185 (94%)	12 (6%)	0	100	100
14	Z	197/219 (90%)	191 (97%)	6 (3%)	0	100	100
15	1	217/273 (80%)	203 (94%)	13 (6%)	1 (0%)	25	62
15	X	217/273 (80%)	199 (92%)	17 (8%)	1 (0%)	25	62
16	2	199/276 (72%)	186 (94%)	13 (6%)	0	100	100
16	Y	199/276 (72%)	185 (93%)	14 (7%)	0	100	100
All	All	7577/8567 (88%)	7194 (95%)	372 (5%)	11 (0%)	50	82

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	232	GLY
15	1	63	SER
15	X	63	SER

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Mol	Chain	Res	Type
9	G	240	PRO
9	G	241	ARG
10	S	116	THR
9	B	103	PRO
9	E	235	GLU
3	g	64	LYS
9	G	239	LYS
13	K	51	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	203/210 (97%)	203 (100%)	0	100	100
1	e	203/210 (97%)	203 (100%)	0	100	100
2	M	186/191 (97%)	186 (100%)	0	100	100
2	f	188/191 (98%)	188 (100%)	0	100	100
3	N	207/221 (94%)	207 (100%)	0	100	100
3	g	207/221 (94%)	207 (100%)	0	100	100
4	O	196/211 (93%)	196 (100%)	0	100	100
4	a	196/211 (93%)	196 (100%)	0	100	100
5	P	196/203 (97%)	195 (100%)	1 (0%)	86	90
5	b	196/203 (97%)	196 (100%)	0	100	100
6	Q	201/225 (89%)	201 (100%)	0	100	100
6	c	201/225 (89%)	201 (100%)	0	100	100
7	R	198/212 (93%)	198 (100%)	0	100	100
7	d	198/212 (93%)	198 (100%)	0	100	100
8	A	183/212 (86%)	183 (100%)	0	100	100
8	D	183/212 (86%)	180 (98%)	3 (2%)	58	74
8	F	185/212 (87%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	B	191/224 (85%)	191 (100%)	0	100	100
9	C	185/224 (83%)	185 (100%)	0	100	100
9	E	186/224 (83%)	186 (100%)	0	100	100
9	G	183/224 (82%)	183 (100%)	0	100	100
10	H	174/175 (99%)	174 (100%)	0	100	100
10	S	174/175 (99%)	173 (99%)	1 (1%)	84	88
11	I	169/171 (99%)	169 (100%)	0	100	100
11	T	168/171 (98%)	168 (100%)	0	100	100
12	J	177/198 (89%)	177 (100%)	0	100	100
12	U	177/198 (89%)	177 (100%)	0	100	100
13	K	178/215 (83%)	177 (99%)	1 (1%)	84	88
13	V	177/215 (82%)	175 (99%)	2 (1%)	70	80
14	W	153/167 (92%)	153 (100%)	0	100	100
14	Z	153/167 (92%)	153 (100%)	0	100	100
15	1	170/216 (79%)	170 (100%)	0	100	100
15	X	170/216 (79%)	170 (100%)	0	100	100
16	2	166/222 (75%)	166 (100%)	0	100	100
16	Y	166/222 (75%)	166 (100%)	0	100	100
All	All	6444/7206 (89%)	6436 (100%)	8 (0%)	92	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	P	134	SER
8	D	234	GLU
8	D	237	SER
8	D	238	MET
13	K	94	THR
10	S	116	THR
13	V	51	VAL
13	V	52	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	53	GLN
1	L	68	HIS
1	L	123	GLN
1	L	150	GLN
2	M	52	GLN
2	M	71	HIS
2	M	119	GLN
3	N	95	GLN
3	N	123	GLN
3	N	155	ASN
4	O	18	GLN
4	O	94	HIS
4	O	205	ASN
5	P	23	GLN
5	P	41	GLN
6	Q	16	GLN
6	Q	43	HIS
6	Q	143	HIS
6	Q	175	HIS
9	B	171	HIS
9	B	173	GLN
8	D	136	ASN
8	D	161	GLN
9	E	164	HIS
9	G	7	GLN
9	G	199	GLN
4	a	18	GLN
4	a	94	HIS
4	a	116	GLN
4	a	122	ASN
5	b	13	ASN
5	b	41	GLN
5	b	73	HIS
5	b	97	GLN
5	b	99	HIS
7	d	144	ASN
7	d	202	HIS
1	e	92	GLN
3	g	100	GLN
3	g	146	GLN
3	g	240	HIS
10	H	7	ASN
10	H	33	GLN

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Mol	Chain	Res	Type
10	H	93	ASN
11	I	8	GLN
11	I	101	ASN
12	J	64	HIS
12	J	86	HIS
12	J	105	HIS
12	J	107	ASN
12	J	185	ASN
13	K	47	GLN
13	K	48	ASN
13	K	92	ASN
13	K	126	HIS
10	S	72	ASN
10	S	173	ASN
10	S	188	HIS
12	U	105	HIS
12	U	107	ASN
12	U	179	ASN
12	U	187	GLN
13	V	91	ASN
13	V	114	GLN
13	V	126	HIS
15	X	61	ASN
15	X	191	GLN
16	Y	234	HIS
16	Y	237	HIS
16	Y	269	HIS
15	1	253	GLN
16	2	82	HIS
16	2	110	ASN
16	2	206	HIS
16	2	247	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

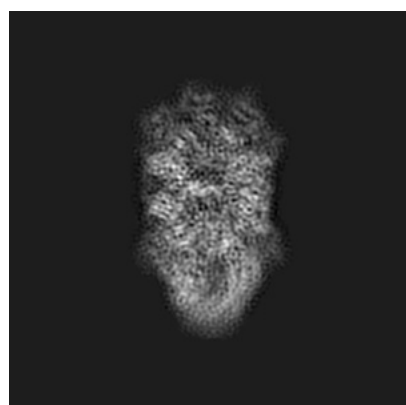
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30824. These allow visual inspection of the internal detail of the map and identification of artifacts.

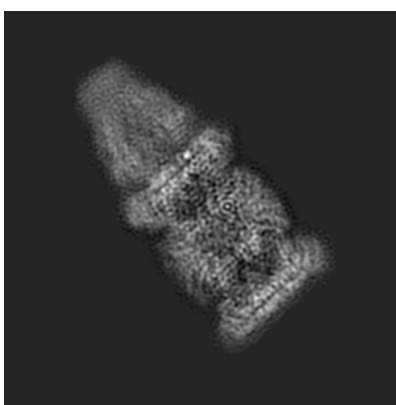
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

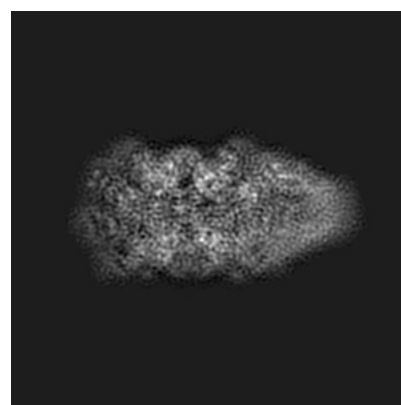
#### 6.1.1 Primary map



X



Y



Z

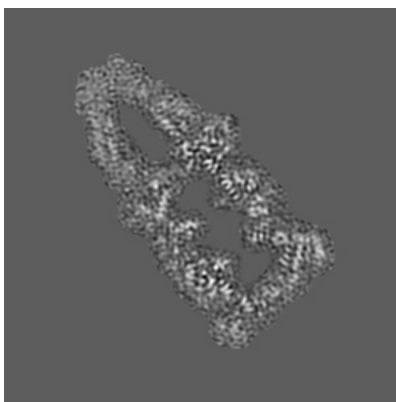
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

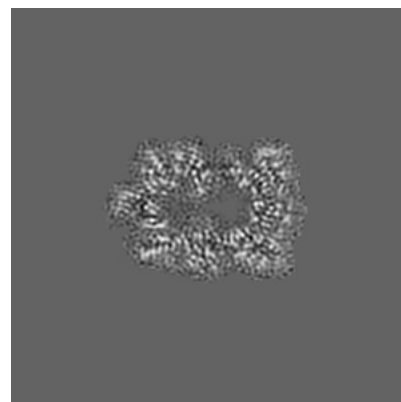
#### 6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

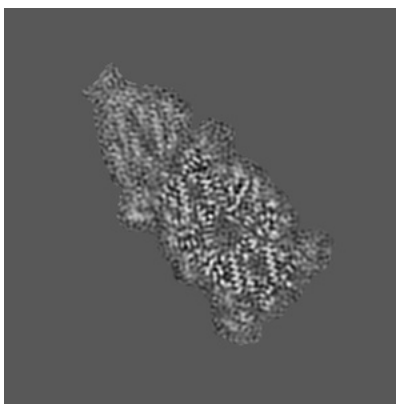
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

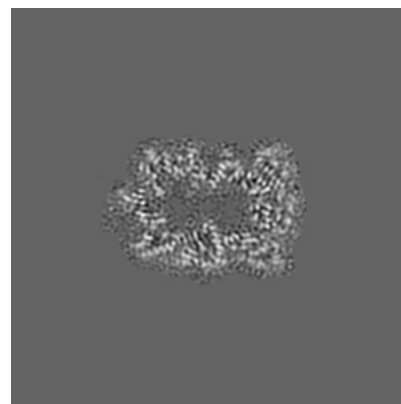
### 6.3.1 Primary map



X Index: 120



Y Index: 109

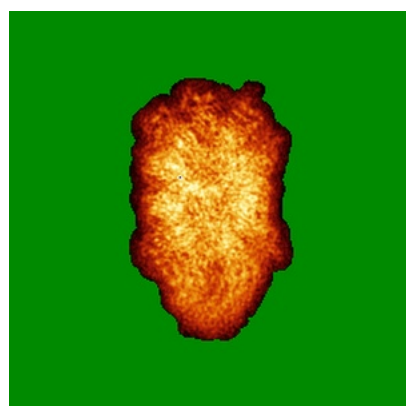


Z Index: 130

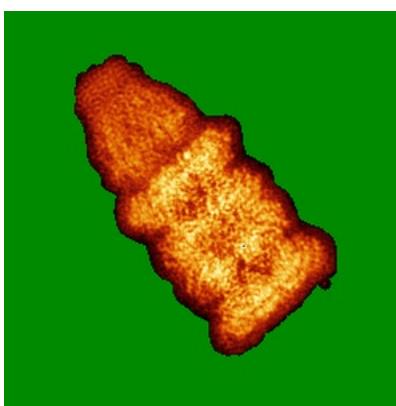
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

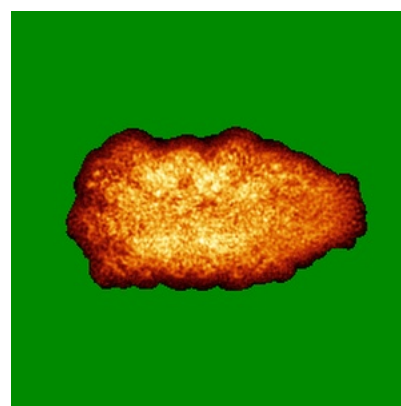
### 6.4.1 Primary map



X



Y

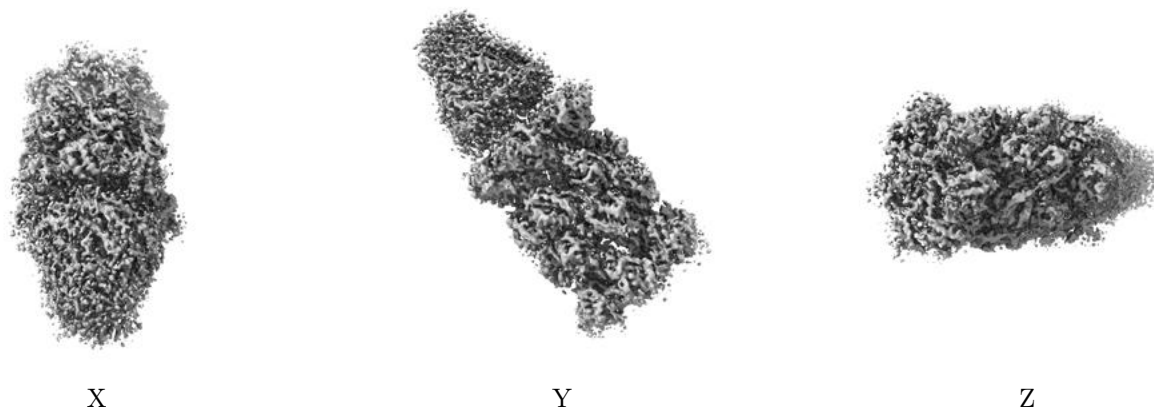


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.619. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

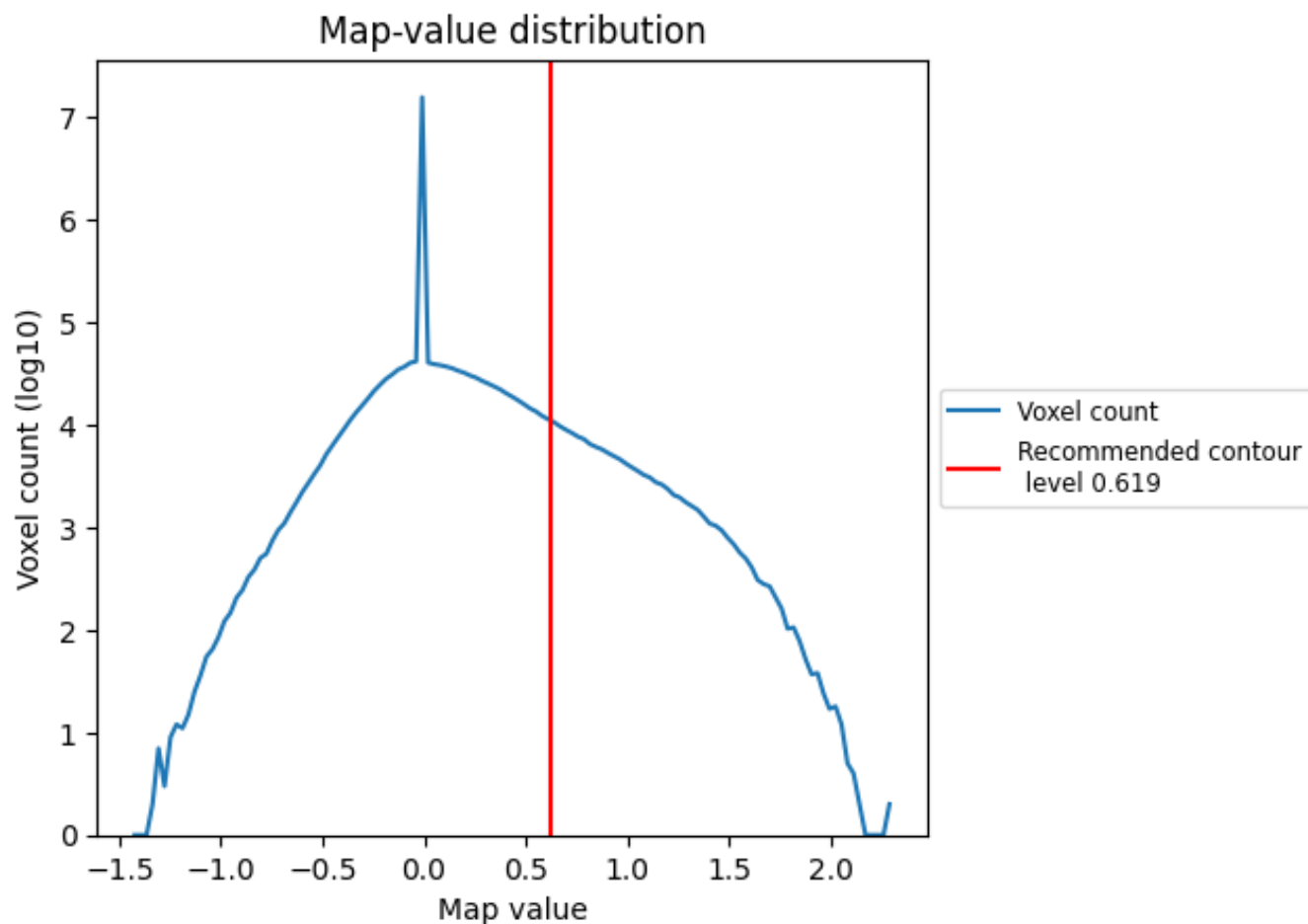
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

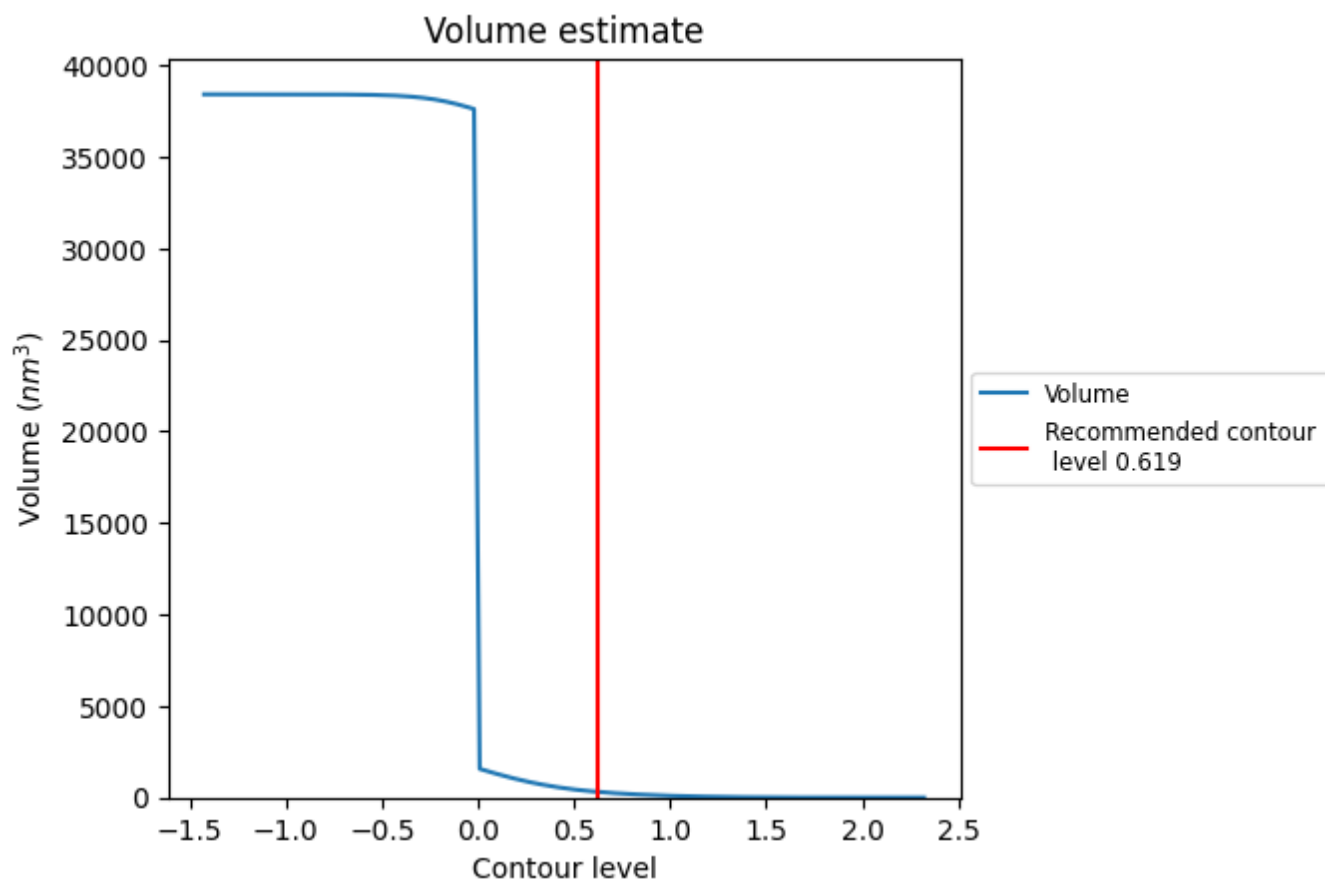
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

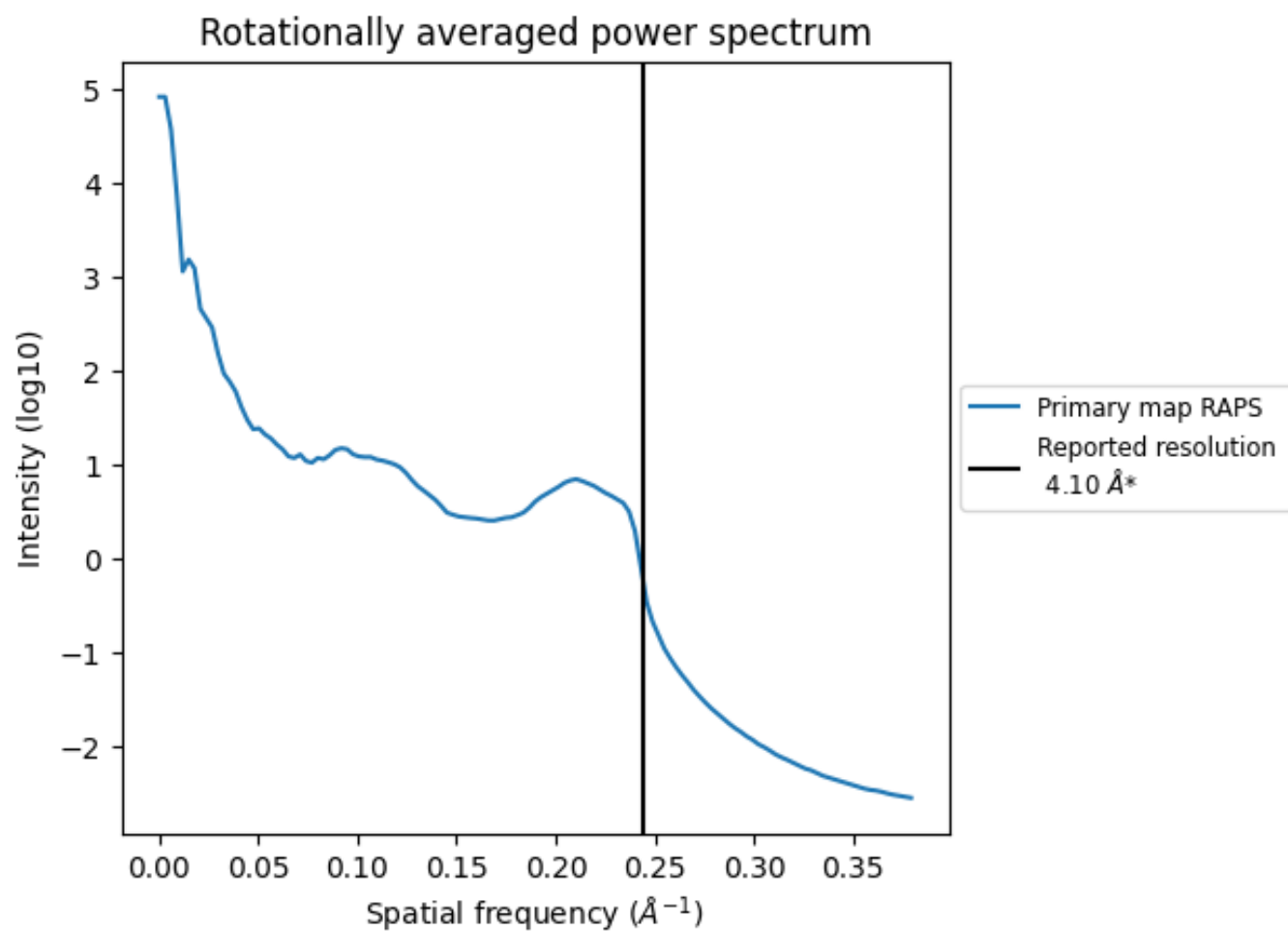
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm<sup>3</sup>; this corresponds to an approximate mass of 285 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

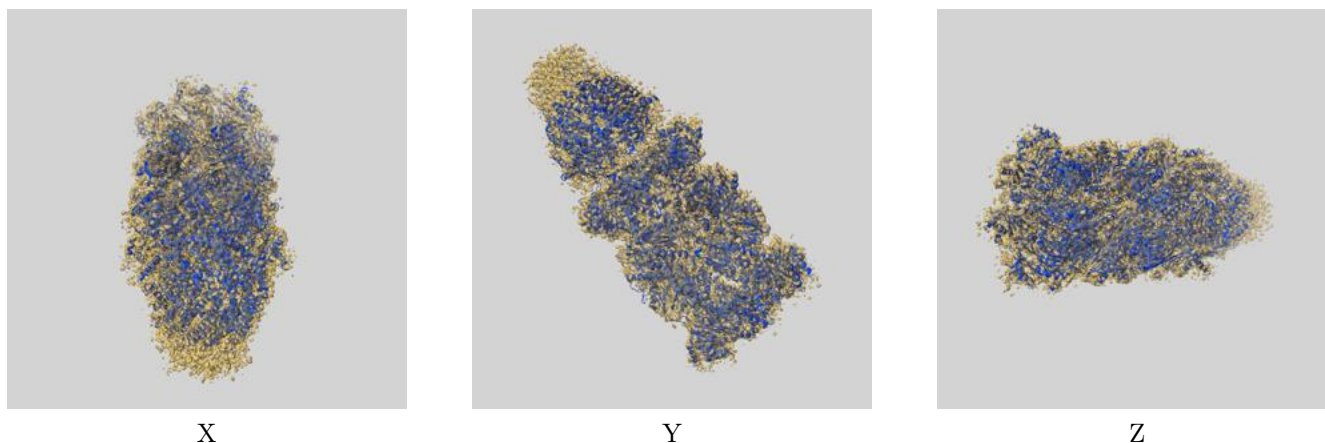
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

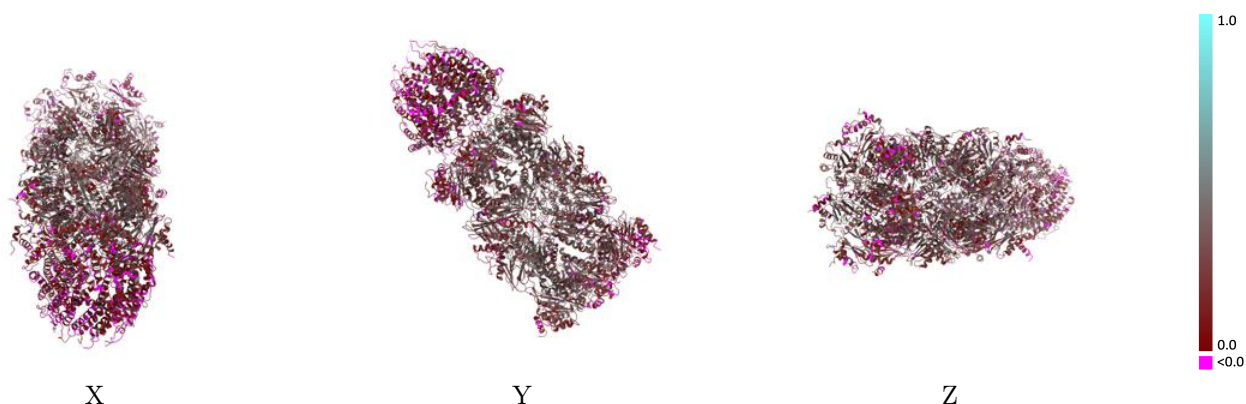
This section contains information regarding the fit between EMDB map EMD-30824 and PDB model 7DR6. Per-residue inclusion information can be found in section [3](#) on page [9](#).

### 9.1 Map-model overlay [i](#)



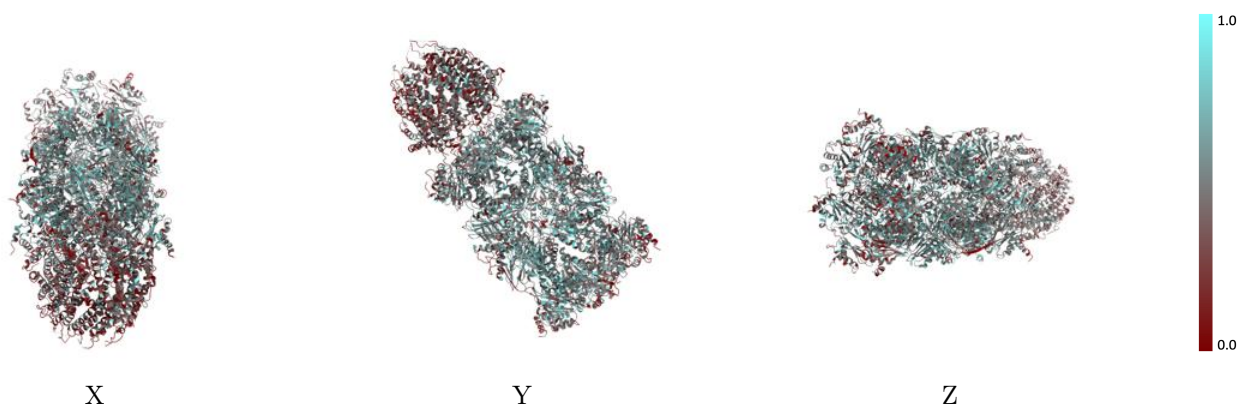
The images above show the 3D surface view of the map at the recommended contour level 0.619 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



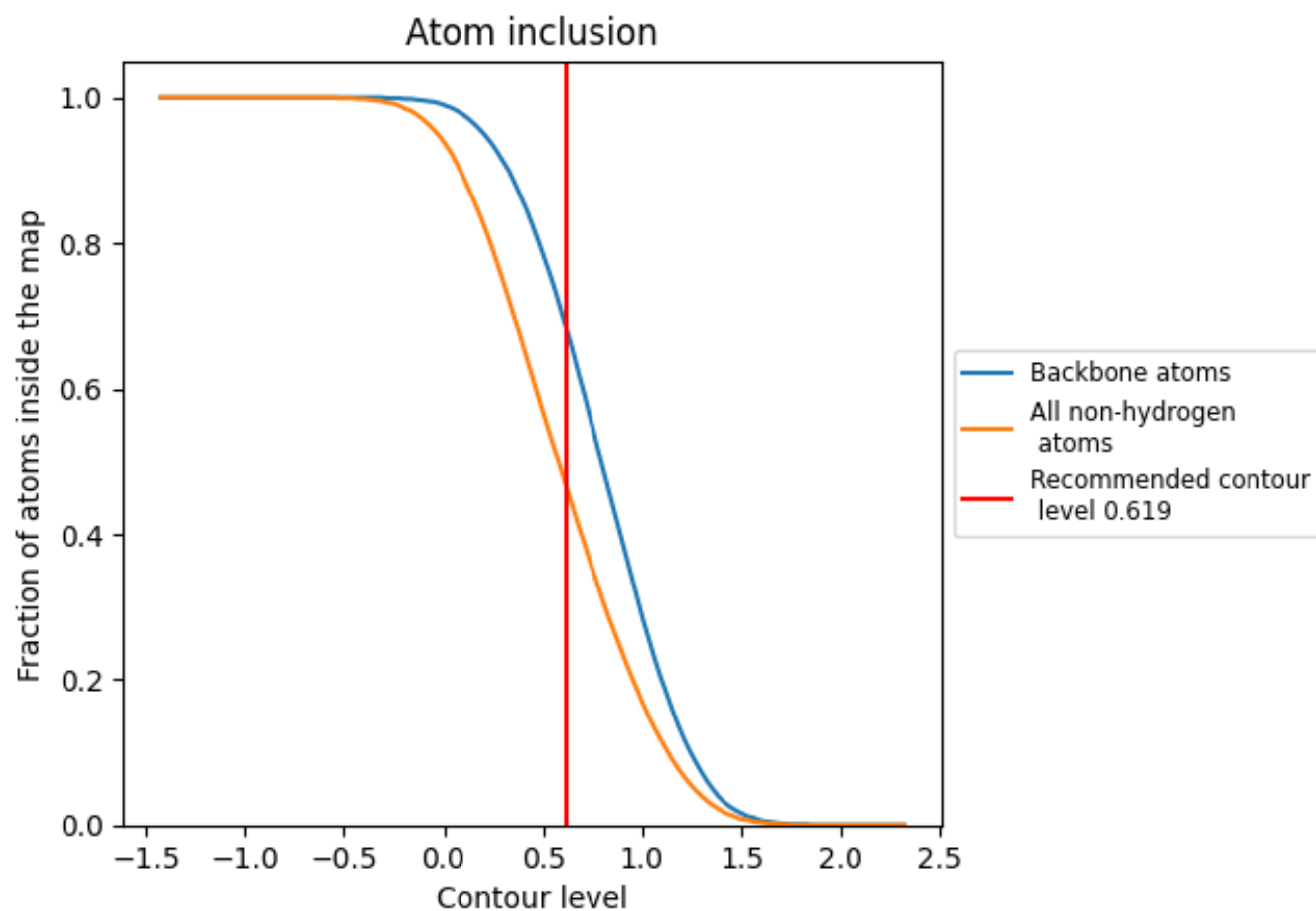
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.619).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.619) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4640	0.2400
1	0.5170	0.2920
2	0.5310	0.2430
A	0.3710	0.1670
B	0.3290	0.1390
C	0.3180	0.1130
D	0.3310	0.1600
E	0.2950	0.1240
F	0.2720	0.0870
G	0.3160	0.1060
H	0.5310	0.3120
I	0.5090	0.2890
J	0.5110	0.2890
K	0.4960	0.2680
L	0.5200	0.2840
M	0.5310	0.2810
N	0.4950	0.2640
O	0.4830	0.2330
P	0.4240	0.1750
Q	0.4840	0.2320
R	0.5150	0.2770
S	0.5300	0.3110
T	0.5300	0.2860
U	0.4910	0.2600
V	0.5050	0.2960
W	0.5490	0.3100
X	0.5140	0.3000
Y	0.5570	0.3170
Z	0.5510	0.2920
a	0.4880	0.2780
b	0.4300	0.2190
c	0.4610	0.2200
d	0.4300	0.1920
e	0.4500	0.2300
f	0.5120	0.2870
g	0.4920	0.2890

